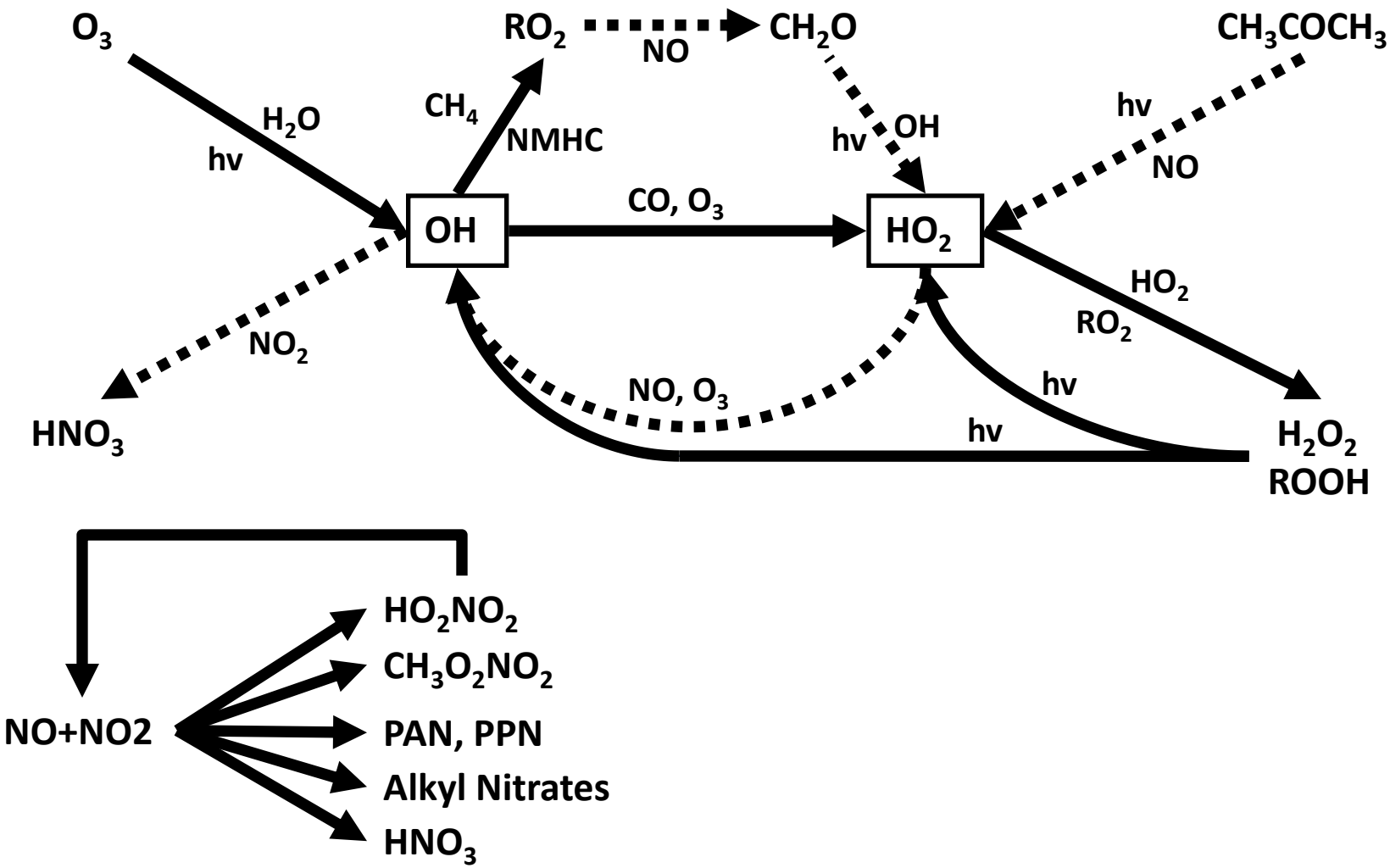
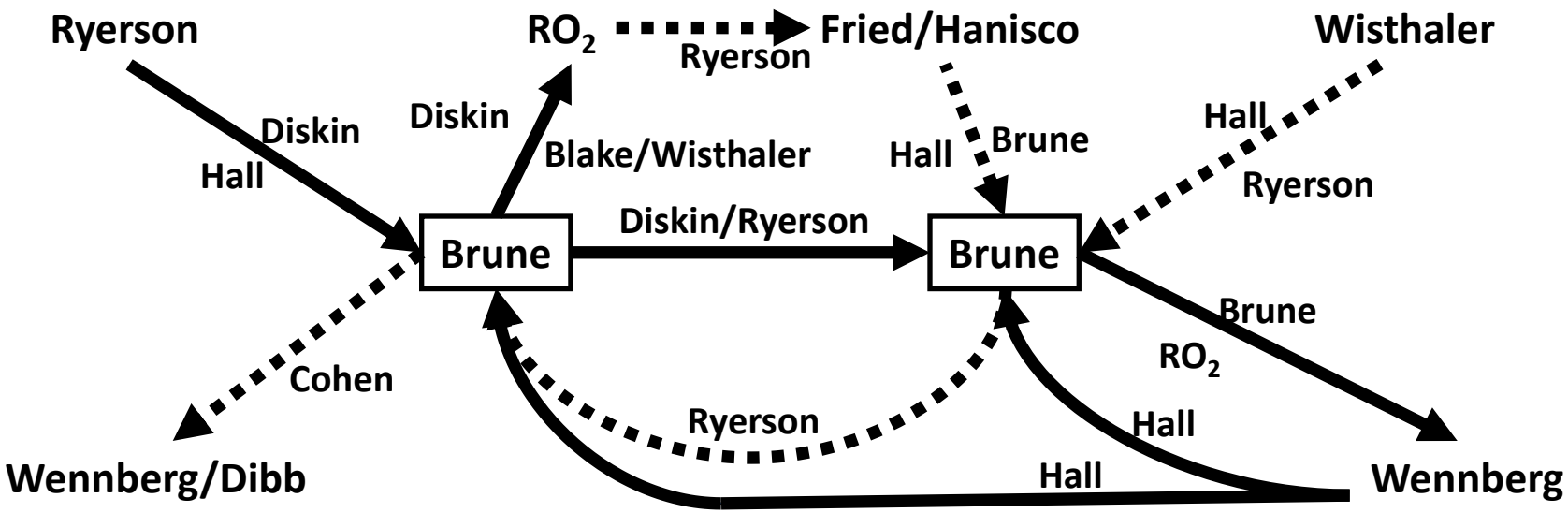
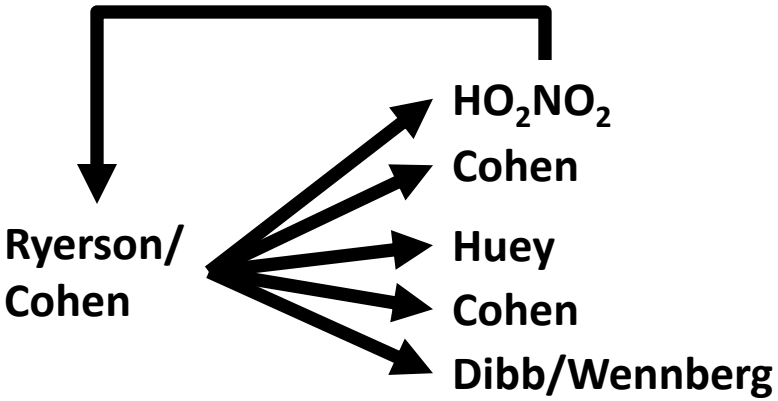
Overview of Ozone Production 0-24 hours after Convection

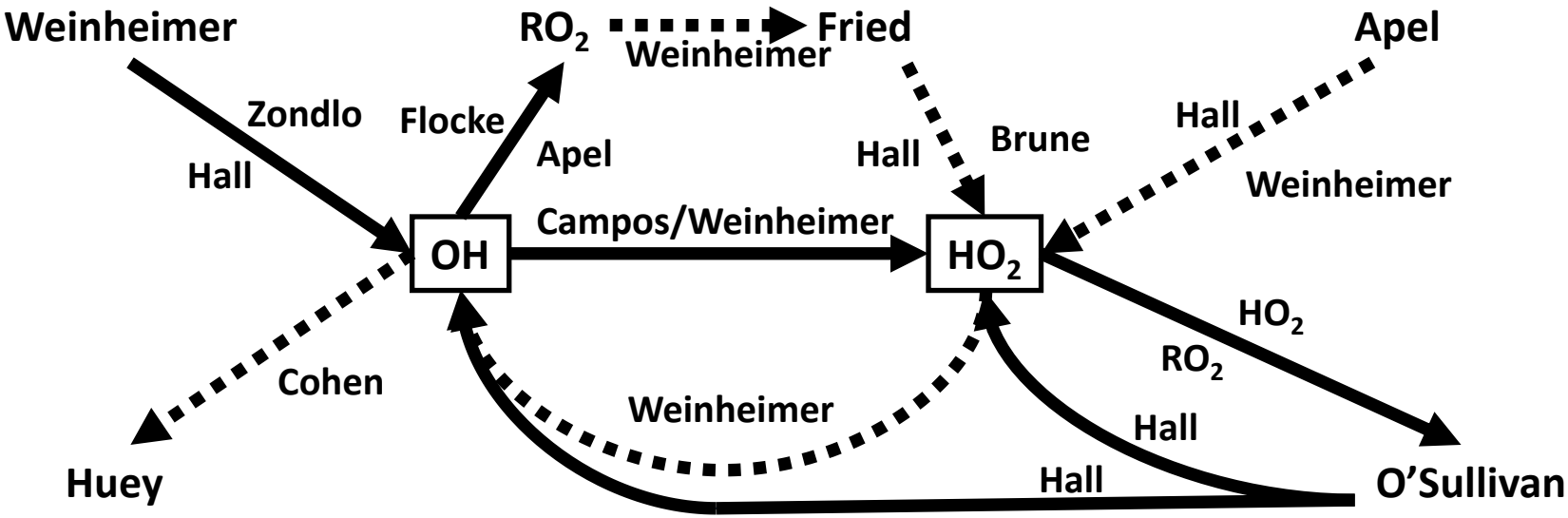


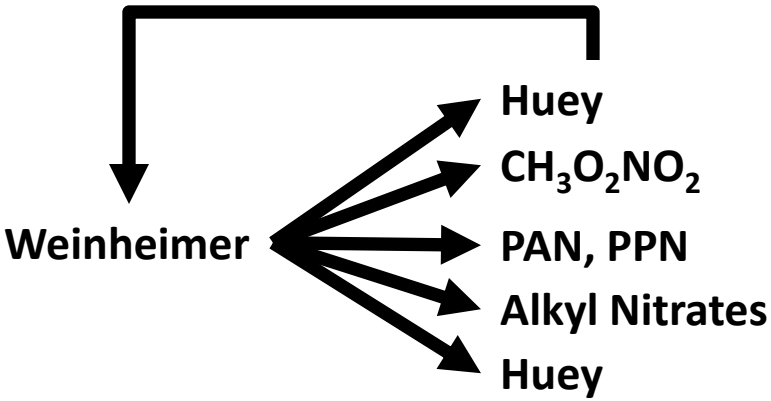
Overview of Ozone Production 0-24 hours after Convection





Overview of Ozone Production 0-24 hours after Convection





Issues and Factors to Consider:

What is the relative importance of lightning produced NOx and convected constituents?

How well do lightning NOx and convected constituents overlap?

How to best capture the impact of mixing and dilution?

How important is mixing with stratospheric or stratospherically-influenced air?

How much material is scavenged by the anvil and released when the anvil dissipates?

Compositional Diagnostics:

Passive Tracers – Fingerprinting and dilution

Short-Lived Species – Photochemical processing rates

Photochemical Products – Ozone production; radical sources, cycling, and reservoirs

Opportunities to examine downwind chemical evolution:

25 May – Oklahoma to 26 May – Illinois Downwind

29 May – Oklahoma to 30 May – Appalachia Downwind

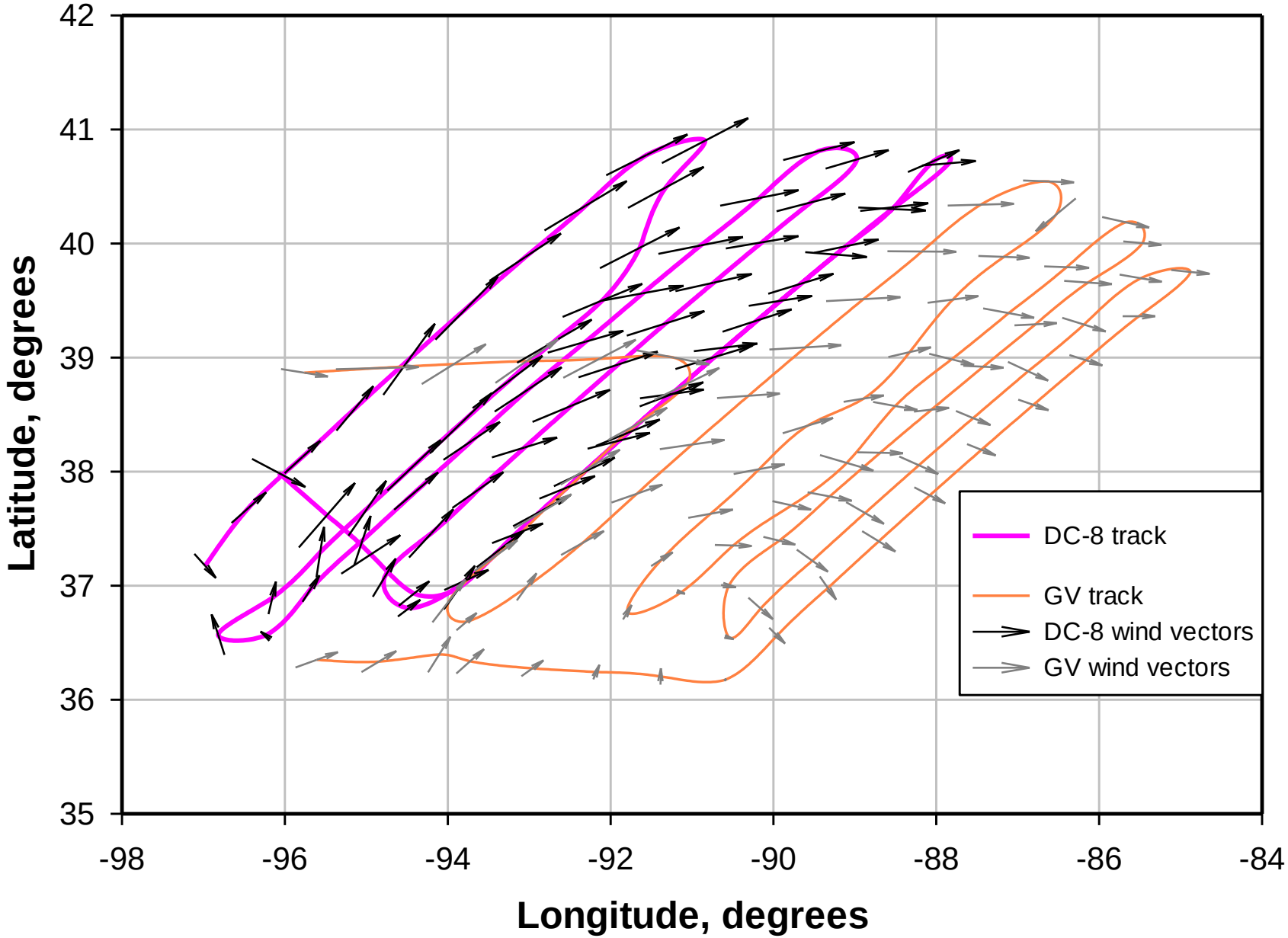
6 June – Colorado to 7 June – Illinois/Missouri Downwind

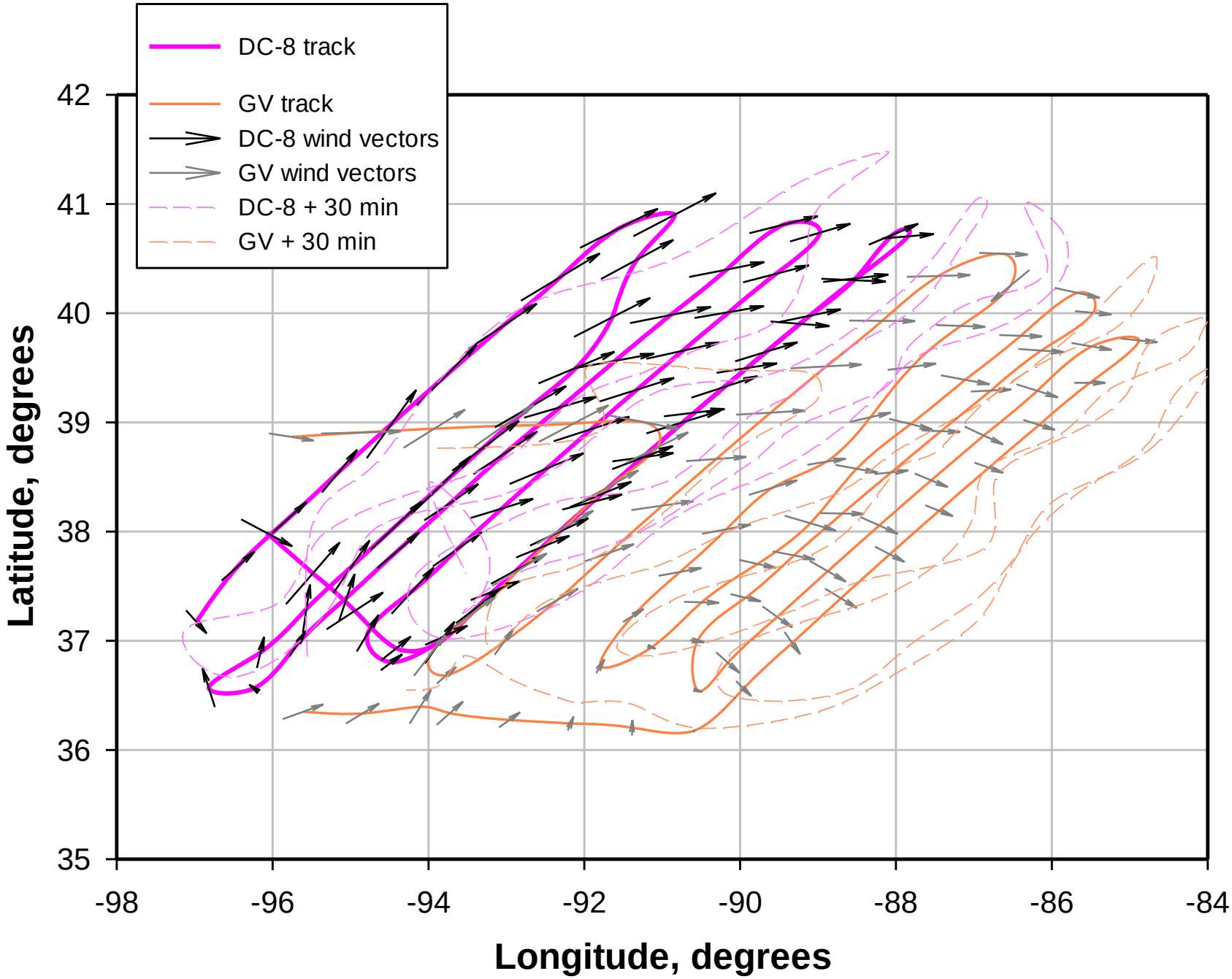
16 June – Oklahoma/Texas to 17 June – Lower Mississippi Valley Downwind

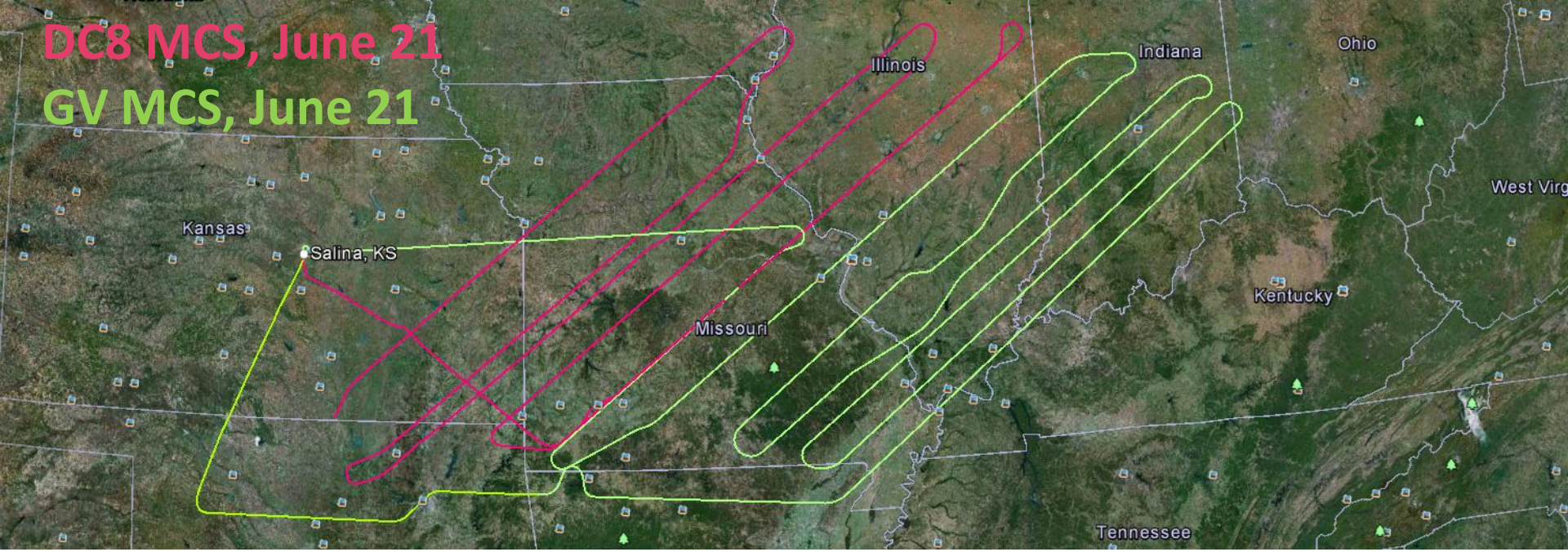
21 June – Lagrangian Sampling of MCS Outflow

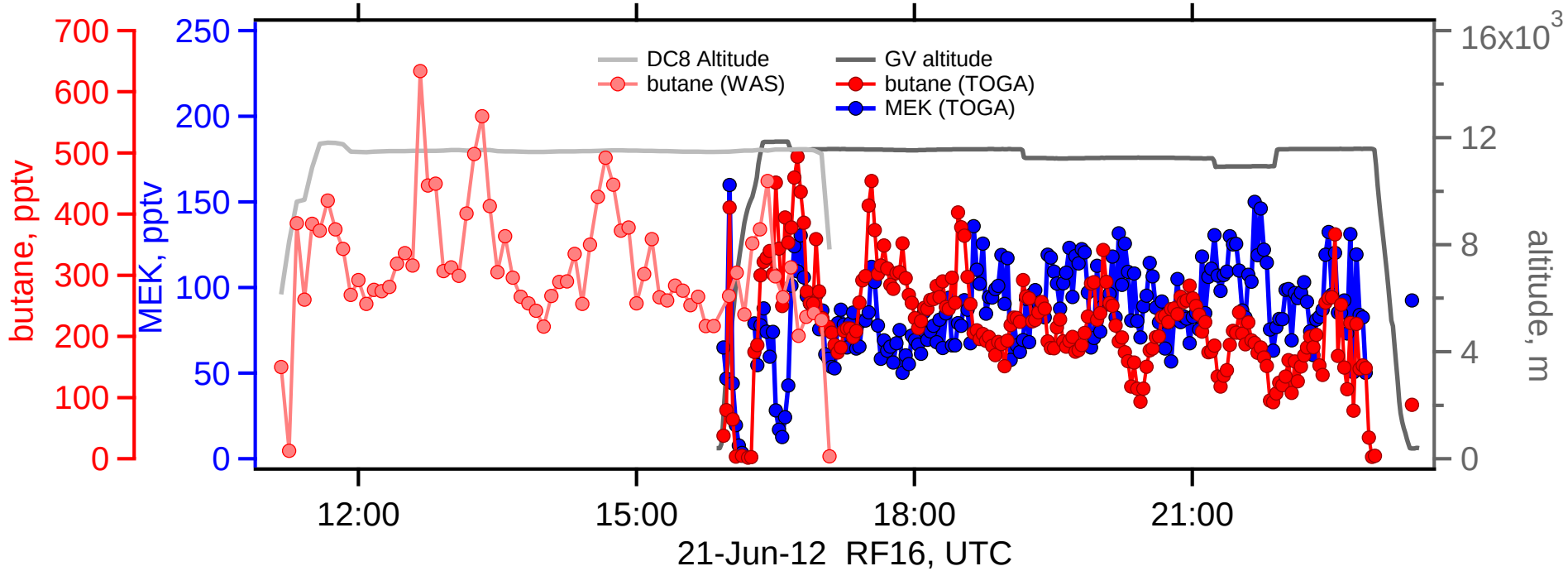
22 June – Colorado to 23 June – Arkansas/Tennessee Downwind

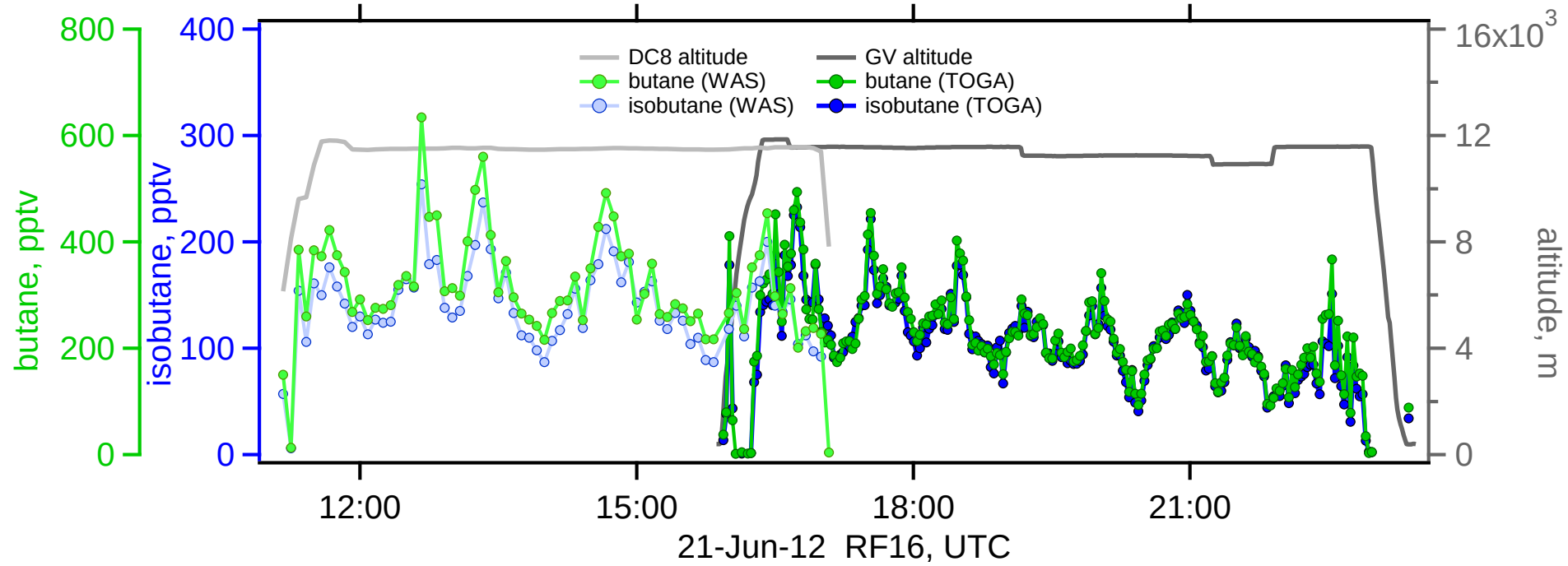
<u>Falcon sampling of Aged Outflow:</u>
8 June – Aged outflow from Colorado located over Kansas
11 June – Two sorties into MCS outflow
17 June – Aged outflow over eastern US on transit to Syracuse

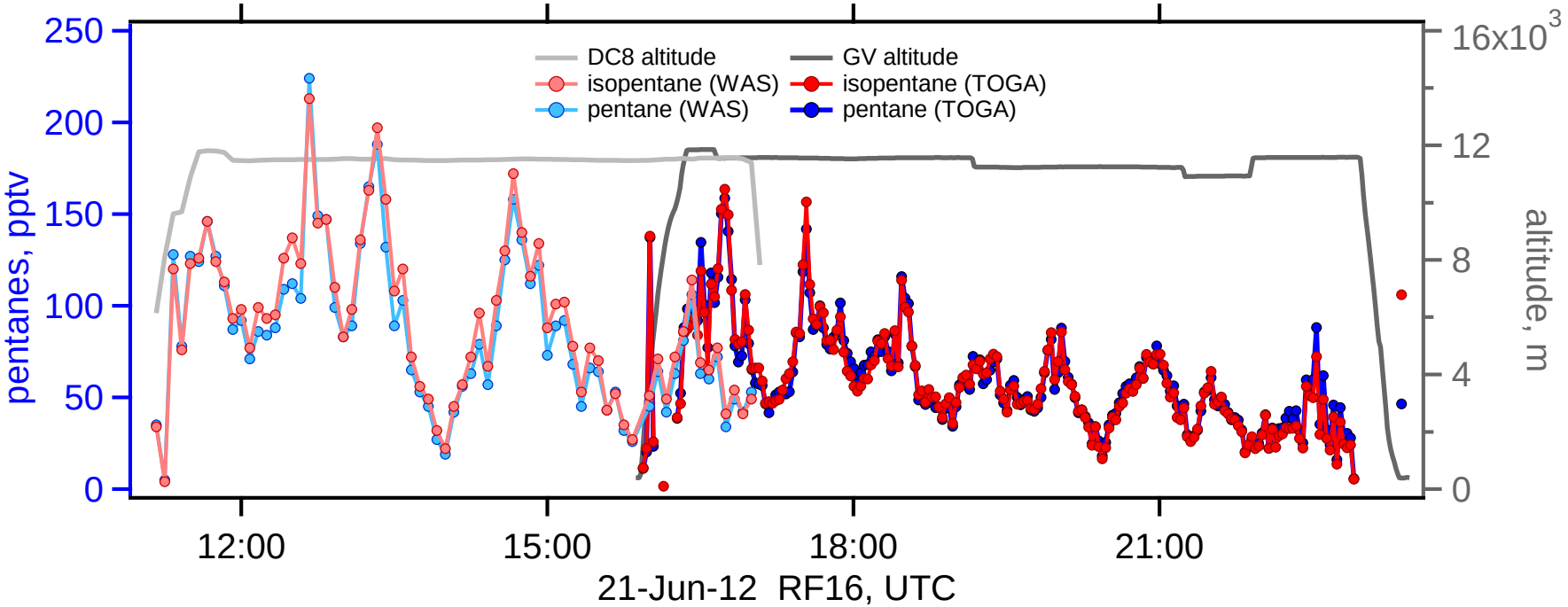

42
41
40
39
38
37
36
35
Latitude, degrees
-98
-96
-94
-92
-90
-88
-86
-84
Longitude, degrees
DC-8 track
GV track
DC-8 wind vectors
GV wind vectors

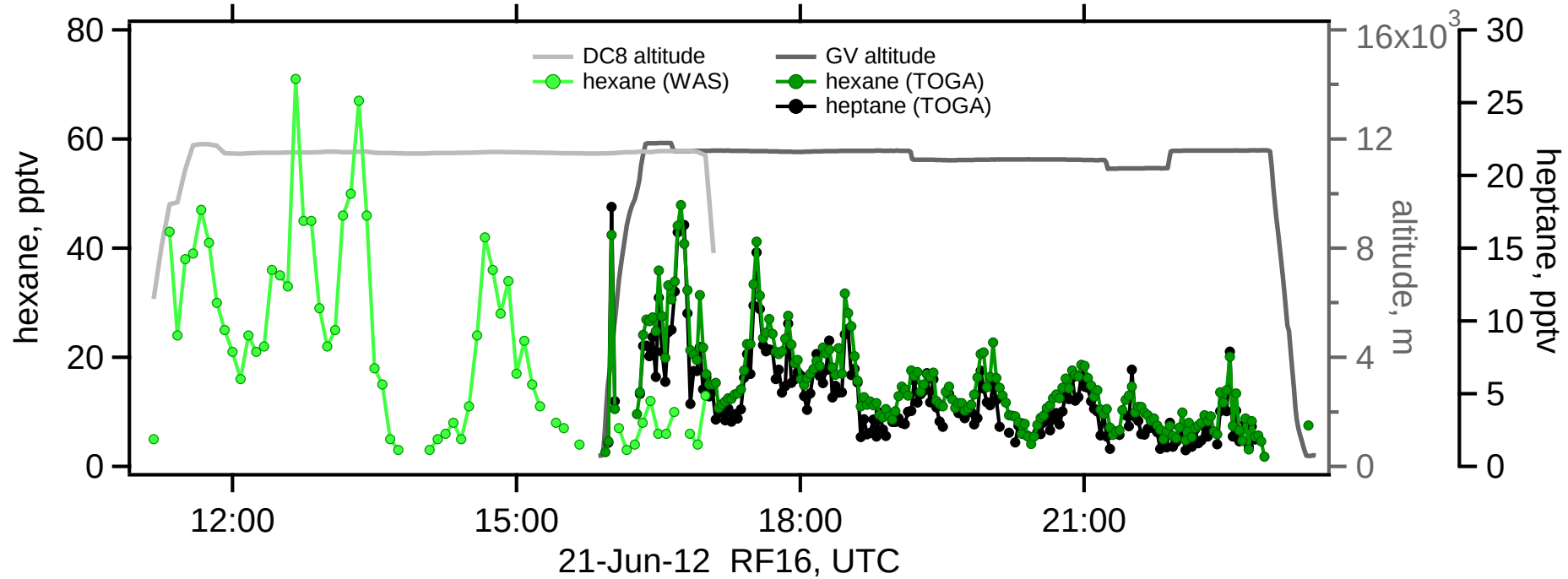

DC-8 track
GV track
DC-8 wind vectors
GV wind vectors
DC-8 + 30 min
GV + 30 min
42
41
40
39
38
37
36
35
Latitude, degrees
-98
-96
-94
-92
-90
-88
-86
-84
Longitude, degrees

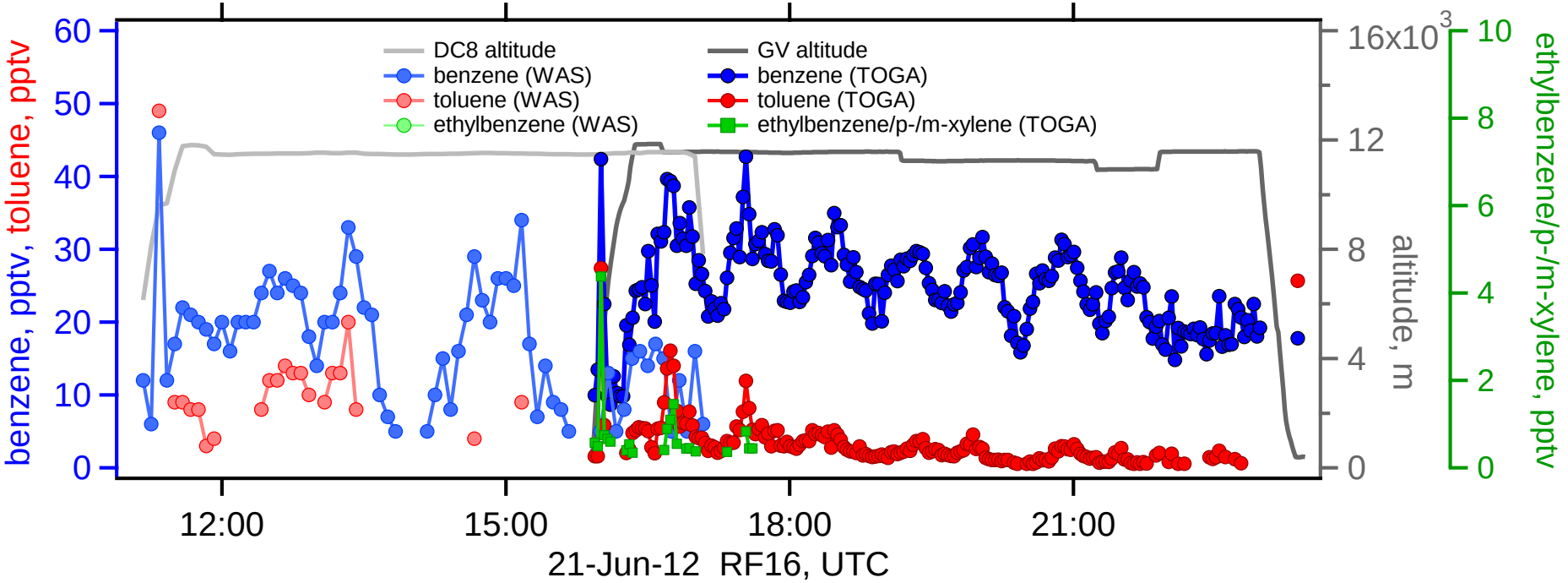

DC8 MCS, June 21
GV MCS, June 21
Kansas
Salina, KS
Missouri
Illinois
Indiana
Ohio
Kentucky
Tennessee

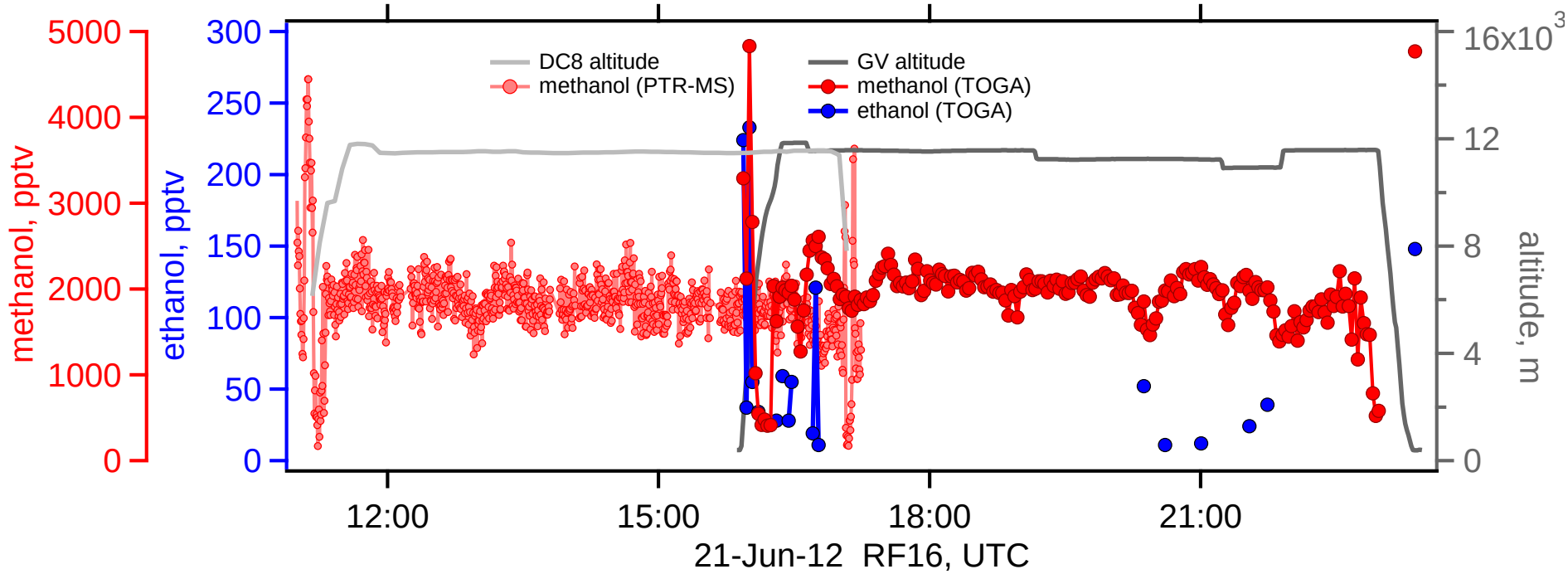

butane, pptv
MEK, pptv
altitude, m
16x10^3
DC8 Altitude
butane (WAS)
GV altitude
butane (TOGA)
MEK (TOGA)
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

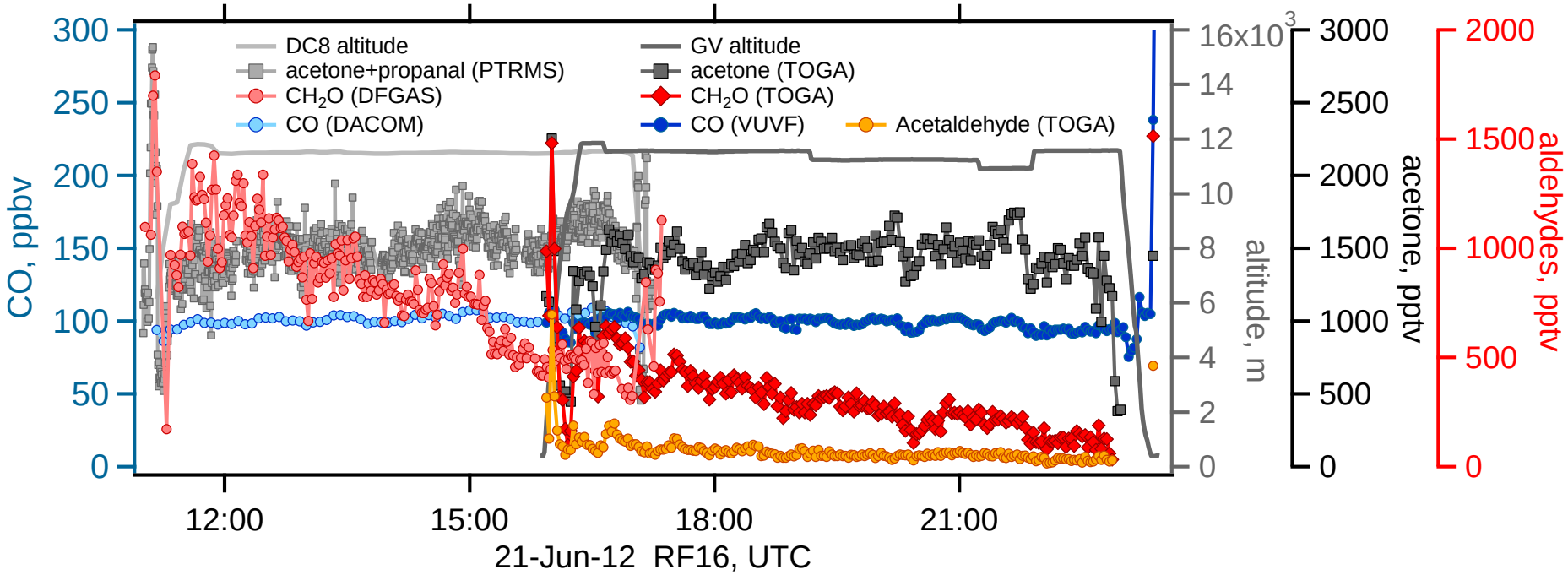

DC8 altitude
butane (WAS)
isobutane (WAS)
GV altitude
butane (TOGA)
isobutane (TOGA)
butane, pptv
isobutane, pptv
altitude, m
16x10^3
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

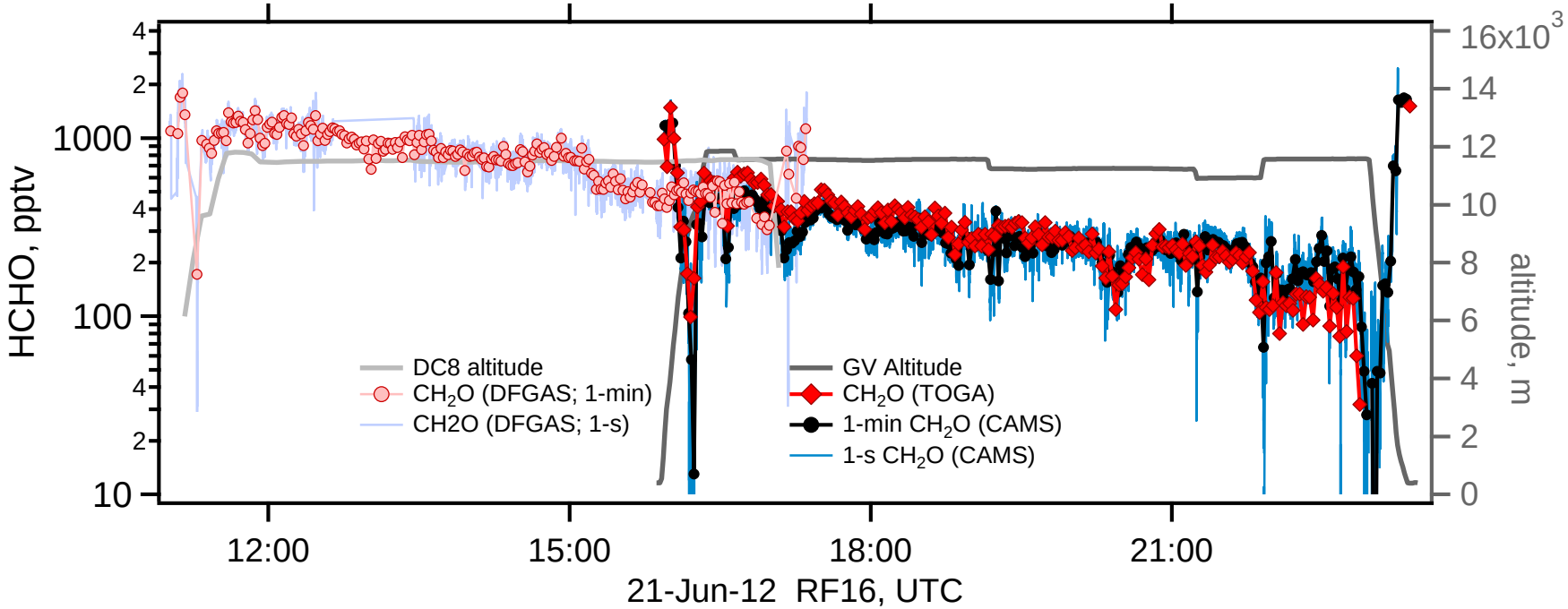

DC8 altitude
isopentane (WAS)
pentane (WAS)
GV altitude
isopentane (TOGA)
pentane (TOGA)
pentanes, pptv
altitude, m
16x10^3
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

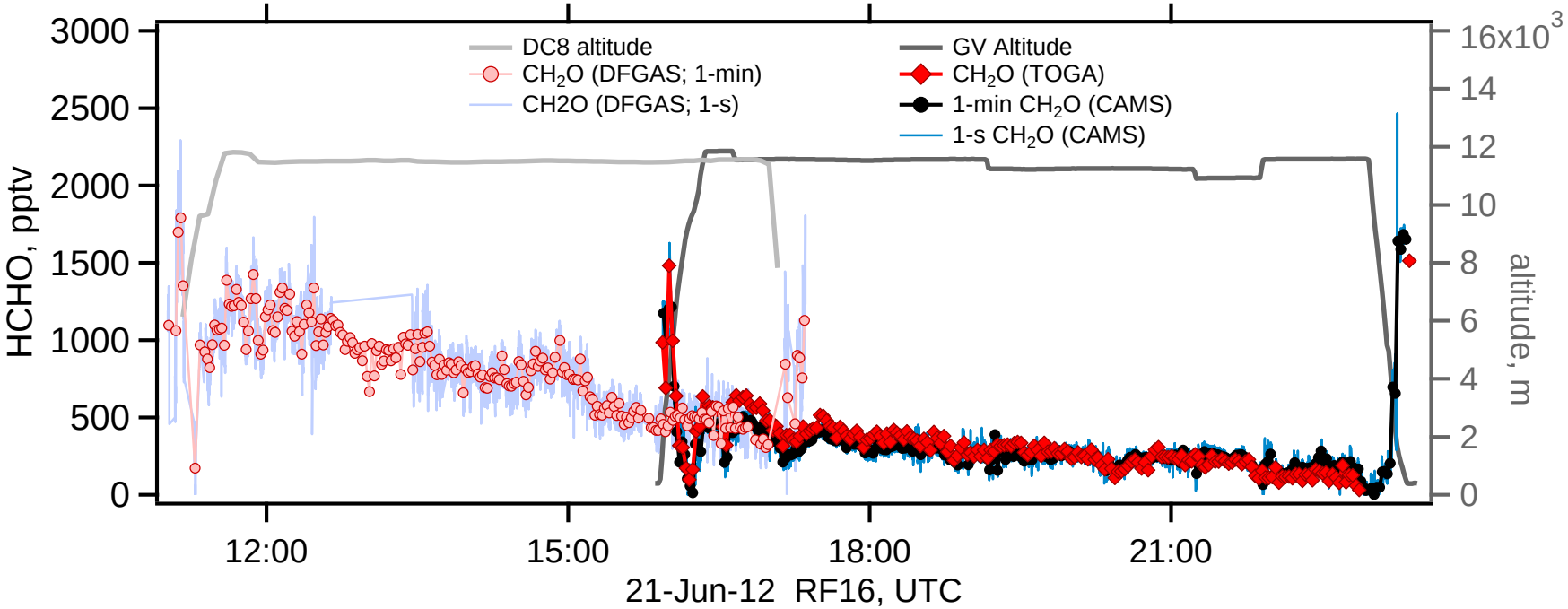

DC8 altitude
hexane (WAS)
GV altitude
hexane (TOGA)
heptane (TOGA)
hexane, pptv
altitude, m
heptane, pptv
16x10^3
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

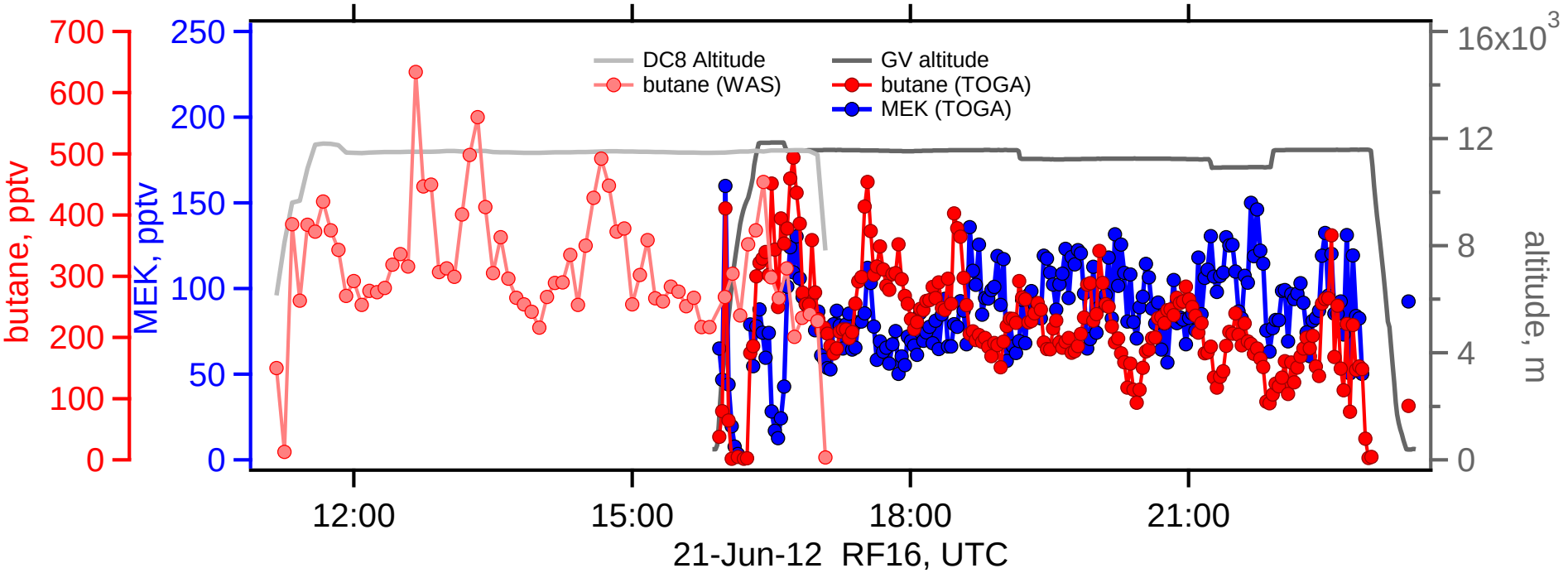

DC8 altitude
benzene (WAS)
toluene (WAS)
ethylbenzene (WAS)
GV altitude
benzene (TOGA)
toluene (TOGA)
ethylbenzene/p-/m-xylene (TOGA)
benzene, pptv, toluene, pptv
altitude, m
ethylbenzene/p-/m-xylene, pptv
16x10^3
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

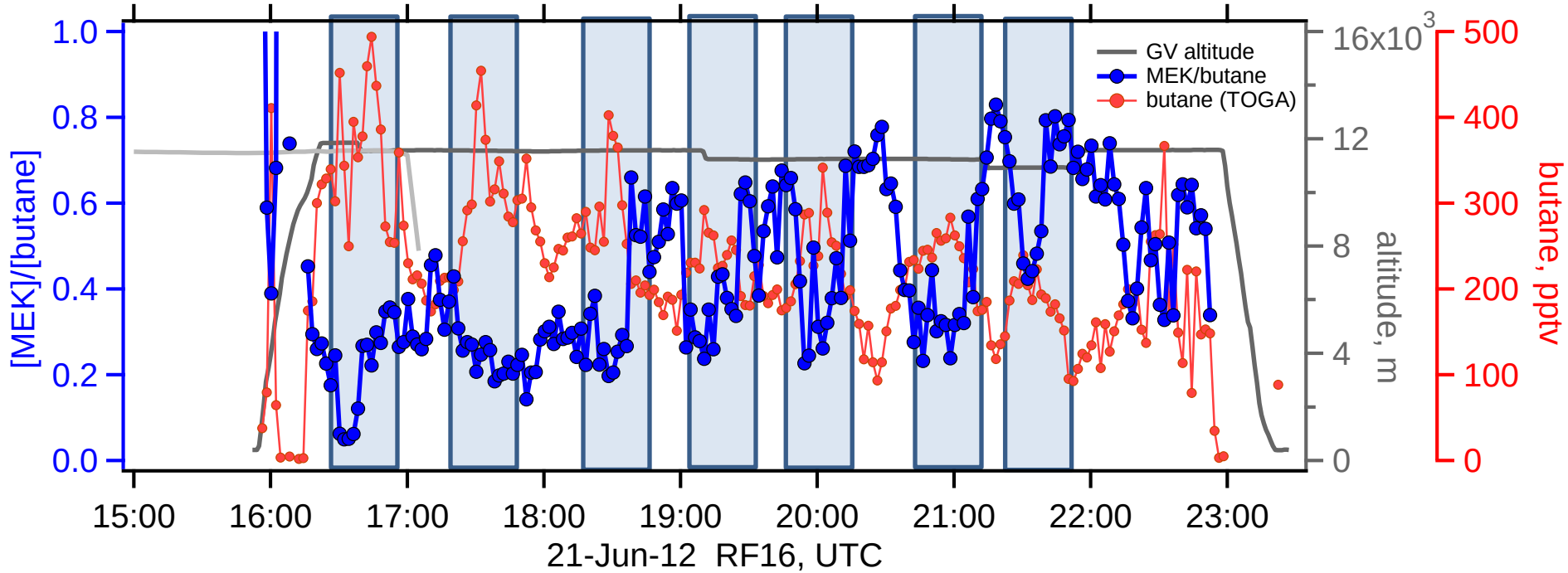

DC8 altitude
methanol (PTR-MS)
GV altitude
methanol (TOGA)
ethanol (TOGA)
methanol, pptv
ethanol, pptv
altitude, m
16x10^3
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

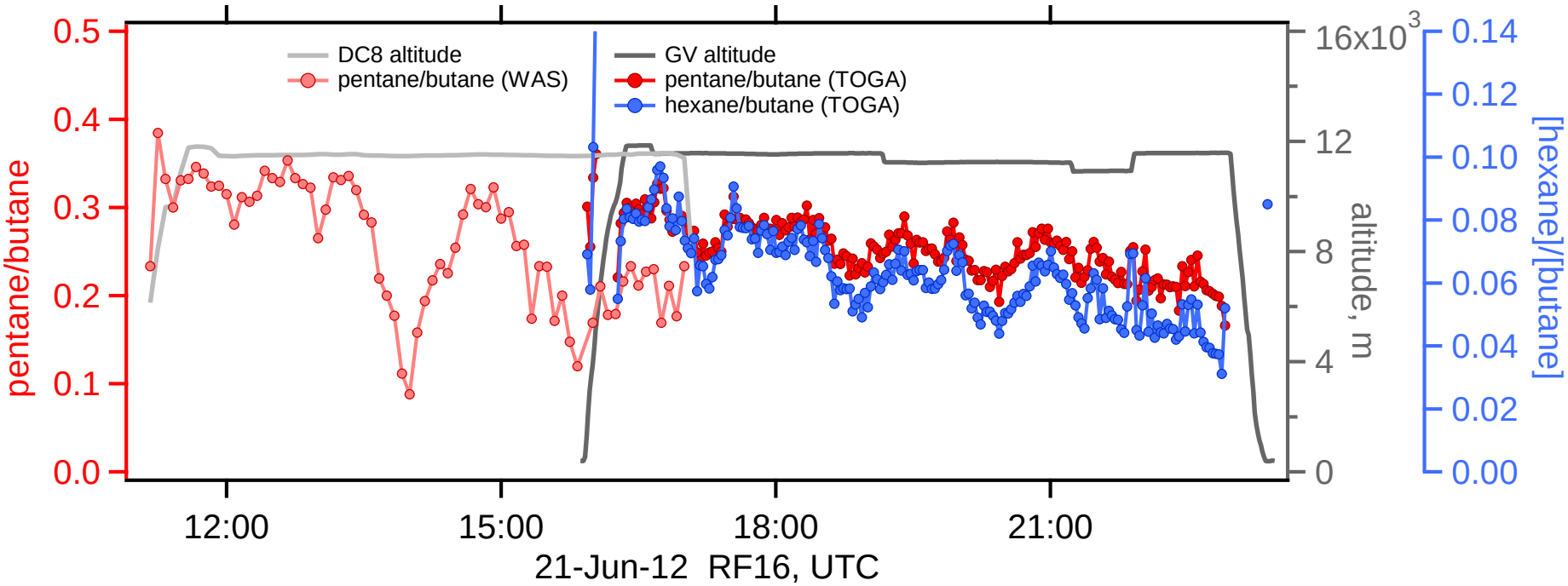

DC8 altitude
acetone+propanal (PTRMS)
CH2O (DFGAS)
CO (DACOM)
GV altitude
acetone (TOGA)
CH2O (TOGA)
CO (VUVF)
Acetaldehyde (TOGA)
CO, ppbv
altitude, m
16x10^3
acetone, pptv
aldehydes, pptv
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

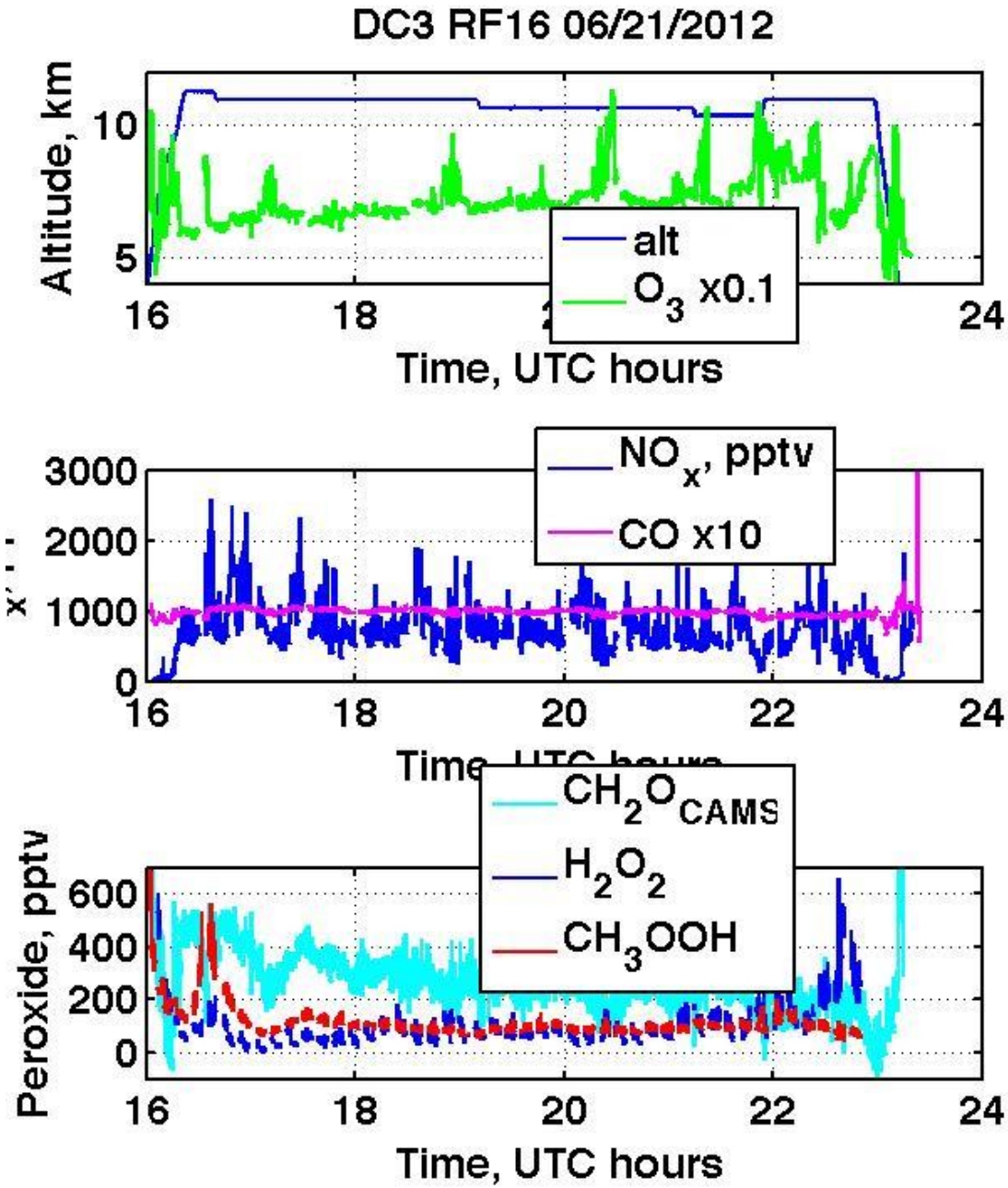

HCHO, pptv
altitude, m
16x10^3
DC8 altitude
CH2O (DFGAS; 1-min)
CH2O (DFGAS; 1-s)
GV Altitude
CH2O (TOGA)
1-min CH2O (CAMS)
1-s CH2O (CAMS)
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC


HCHO, pptv
altitude, m
16x10^3
DC8 altitude
CH2O (DFGAS; 1-min)
CH2O (DFGAS; 1-s)
GV Altitude
CH2O (TOGA)
1-min CH2O (CAMS)
1-s CH2O (CAMS)
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

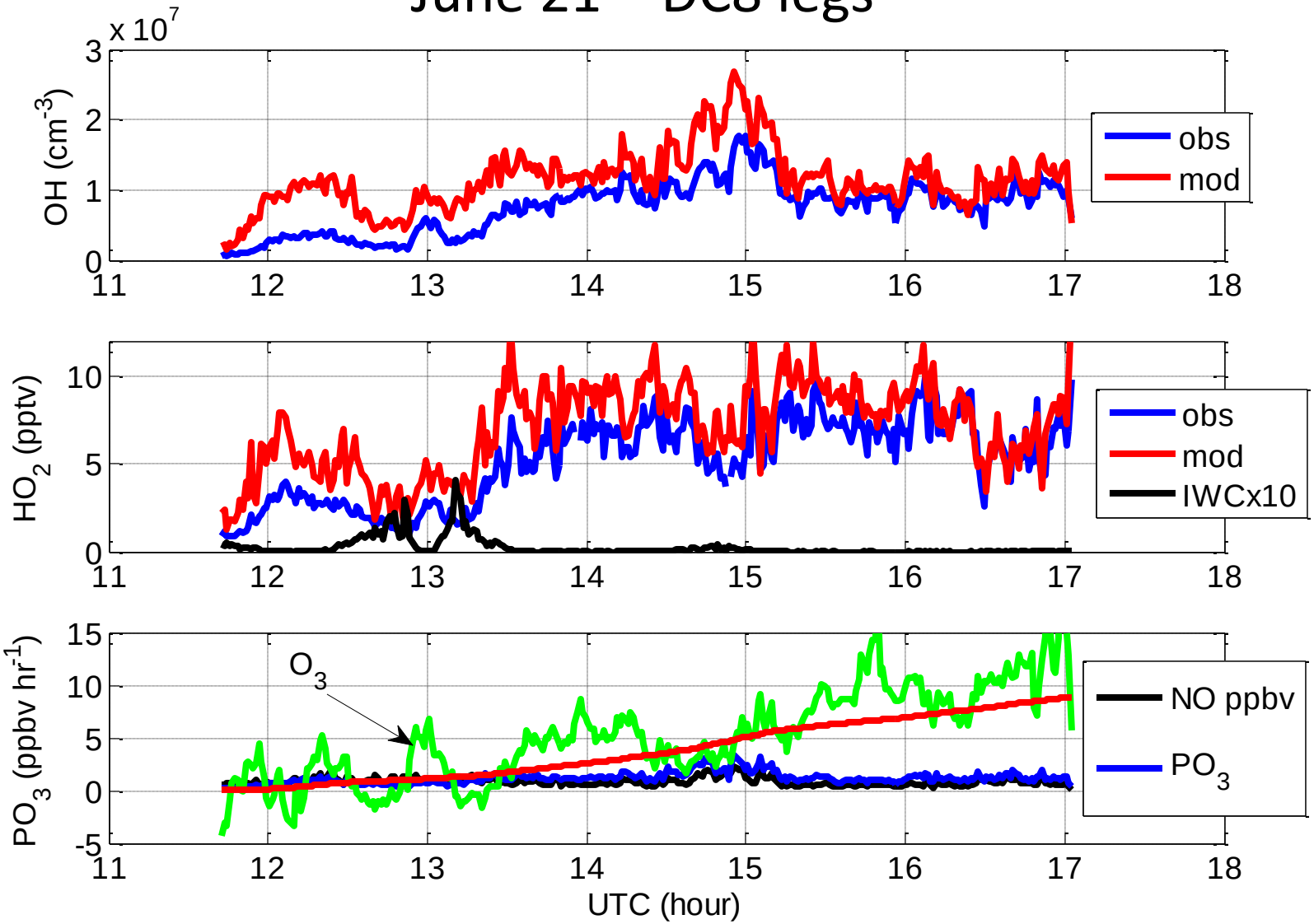

DC8 Altitude
butane (WAS)
GV altitude
butane (TOGA)
MEK (TOGA)
butane, pptv
MEK, pptv
altitude, m
16x10^3
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC


GV altitude
MEK/butane
butane (TOGA)
[MEK]/[butane]
altitude, m
butane, pptv
16x10^3
15:00
16:00
17:00
18:00
19:00
20:00
21:00
22:00
23:00
21-Jun-12 RF16, UTC

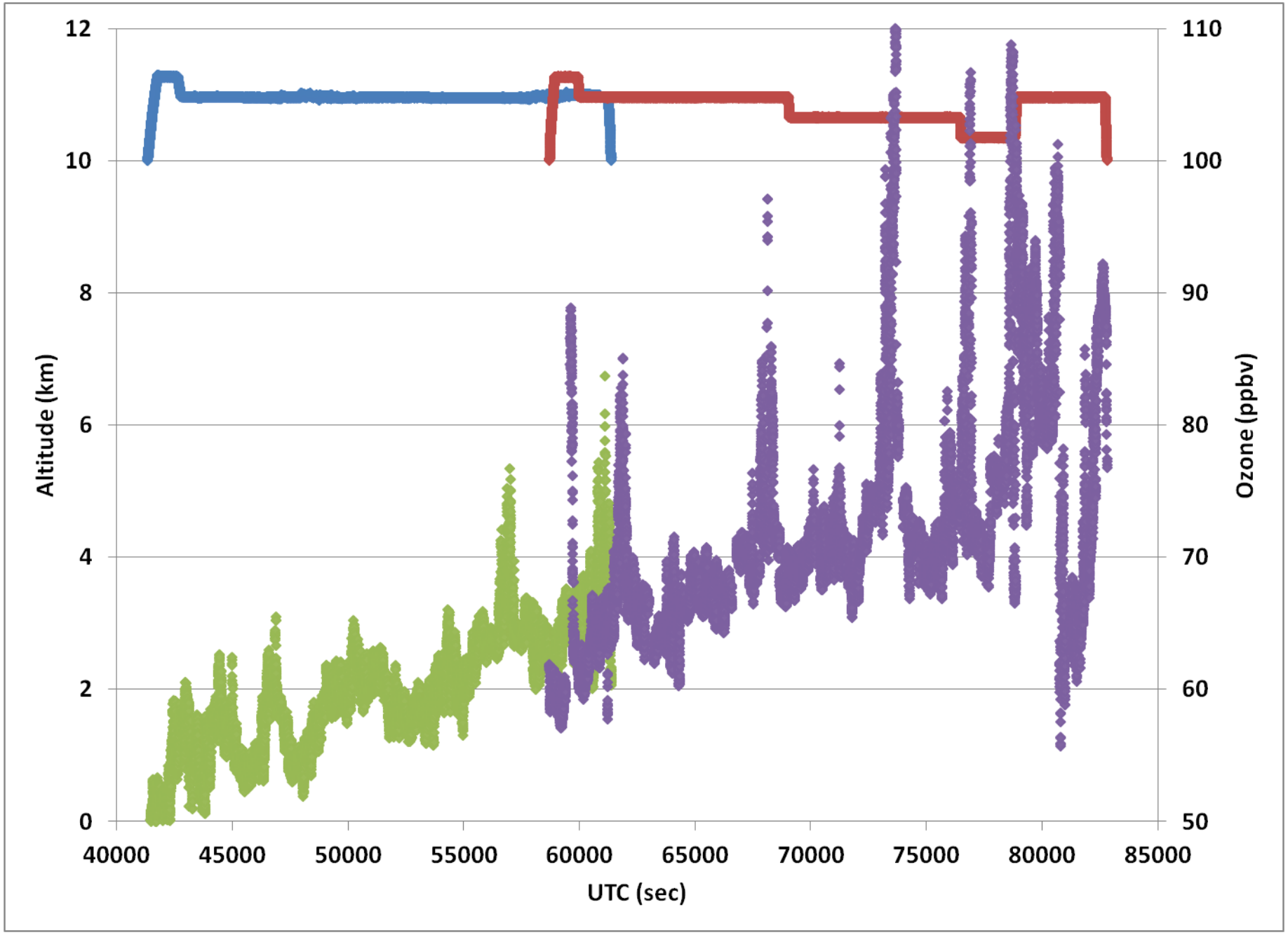

DC8 altitude
pentane/butane (WAS)
GV altitude
pentane/butane (TOGA)
hexane/butane (TOGA)
pentane/butane
0.5
0.4
0.3
0.2
0.1
0.0
16x10^3
12
8
4
0
altitude, m
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
[hexane]/[butane]
12:00
15:00
18:00
21:00
21-Jun-12 RF16, UTC

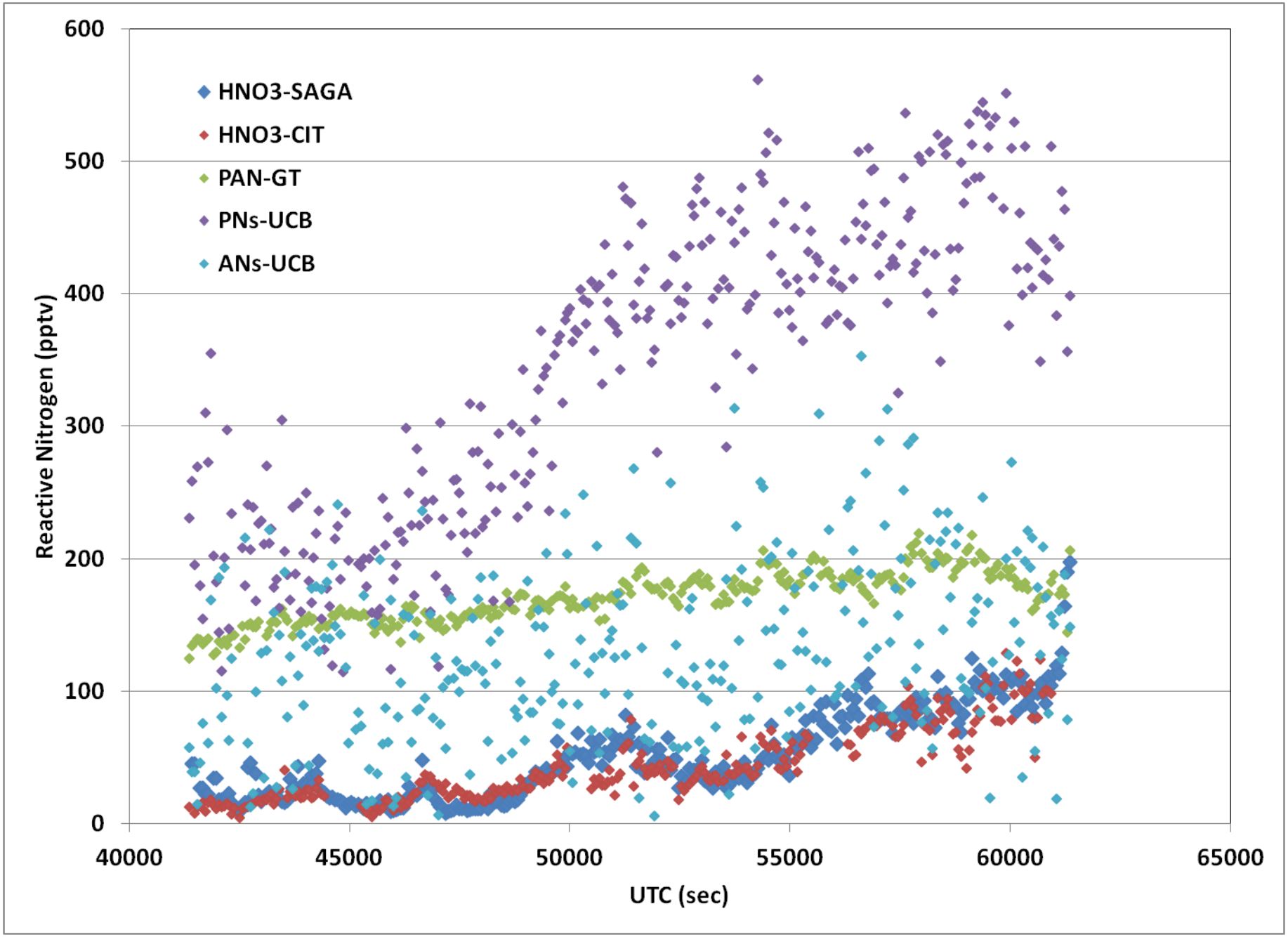

DC3 RF16 06/21/2012
Altitude, km
10
5
16
18
24
alt
O3 x0.1
Time, UTC hours
3000
2000
1000
0
16
18
20
22
24
NOx, pptv
CO x10
Time, UTC hours
Peroxide, pptv
600
400
200
0
16
18
20
22
24
CH2OCAMS
H2O2
CH3OOH
Time, UTC hours

June 21 – DC8 legs

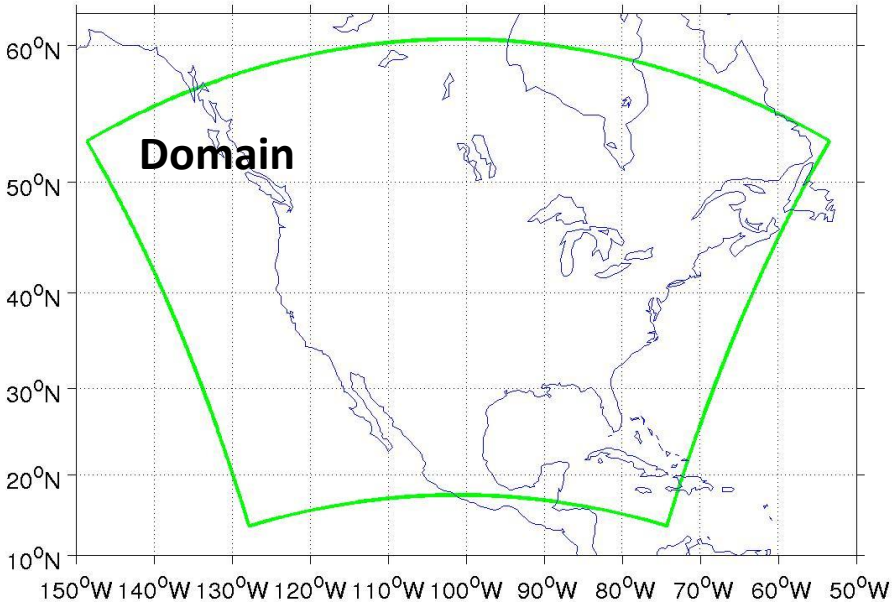


- modeled HOx > measured HOx in cirrus at beginning
- PO_3 calculated from measured HO_2 + modeled RO_2
- PO_3 appears to be NO_x-limited


12
10
8
6
4
2
0
Altitude (km)
110
100
90
80
70
60
50
Ozone (ppbv)
40000
45000
50000
55000
60000
65000
70000
75000
80000
85000
UTC (sec)


HNO3-SAGA
HNO3-CIT
PAN-GT
PNs-UCB
ANs-UCB
Reactive Nitrogen (pptv)
0
100
200
300
400
500
600
40000
45000
50000
55000
60000
65000
UTC (sec)

WRF-Chem Storm/Downwind Flight Simulations (Bela, Barth)



Grid spacing: dx = 15 km, 40 vertical levels to 50 hPa (~650 m in UT)

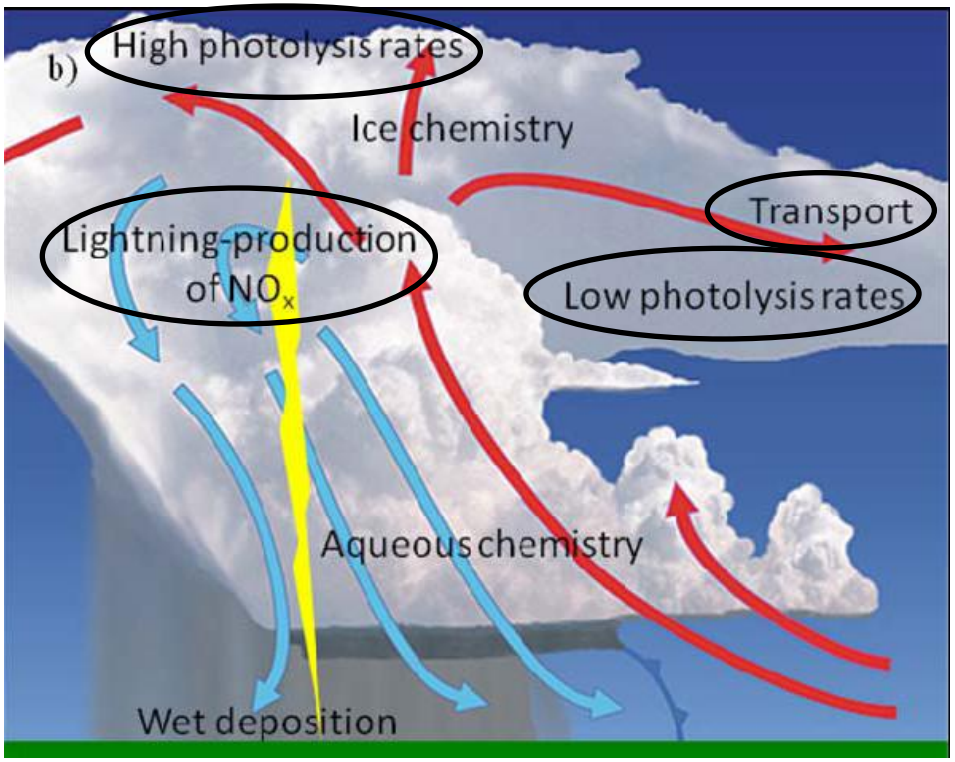
Initial/Boundary Conditions: DART (met), MOZART (chem)

Physics: Grell 3D convection, Morrison cloud microphysics, MYJ PBL

Chemistry: MOZART gas chemistry mechanism; GOCART aerosol scheme

Emissions: EPA NEI 2005 anthropogenic (2012 NO/NO2 based on OMI NO2), aircraft from Baughcum (1999), MEGAN v2.0.4 biogenic, FINN fire

Included processes:



https://www2.acd.ucar.edu/sites/default/files/dc3/thunderstorm-airmass_squall-line.jpg

Lightning-NOx : FR = $3.44 \times 10^{-5}\ z_{top}^{4.9}$

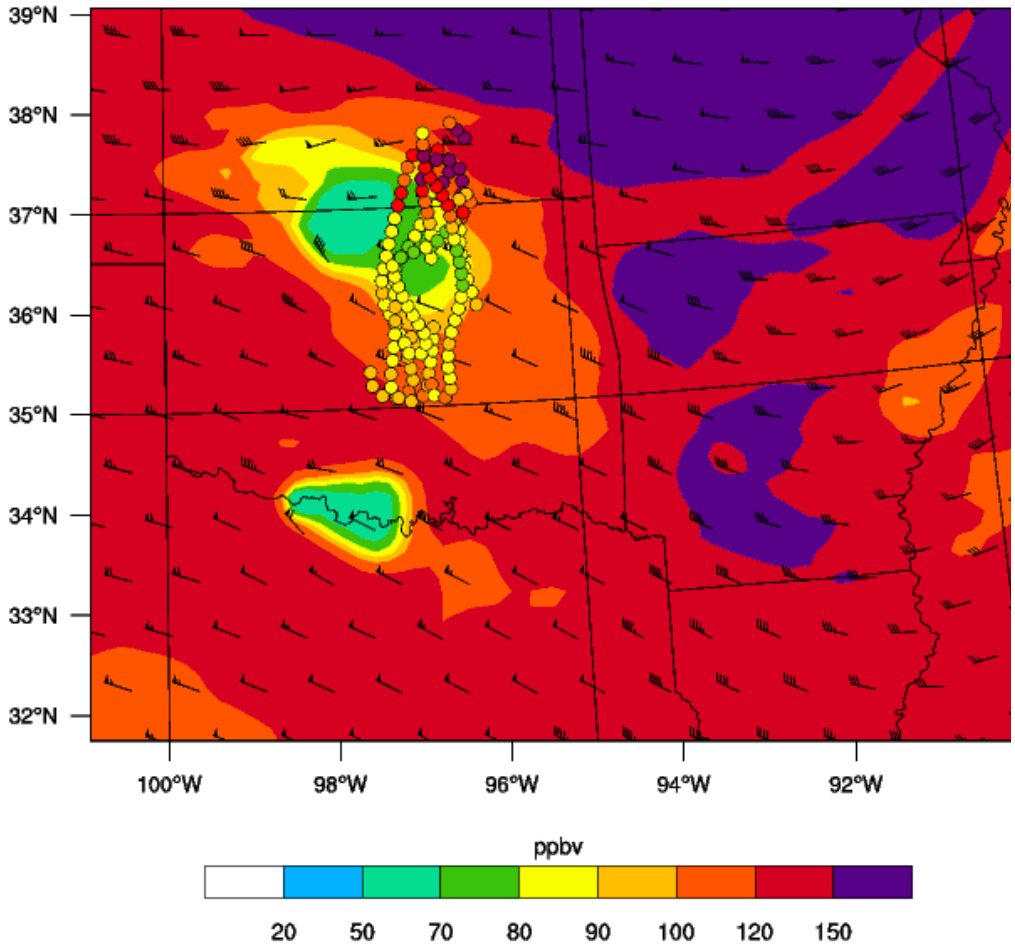
z_{top} = cloud top height = level neutral buoyancy – 2 km (Wong et al., 2012)

500 moles NO/flash placed vertically following Ott et al. (2010) curves

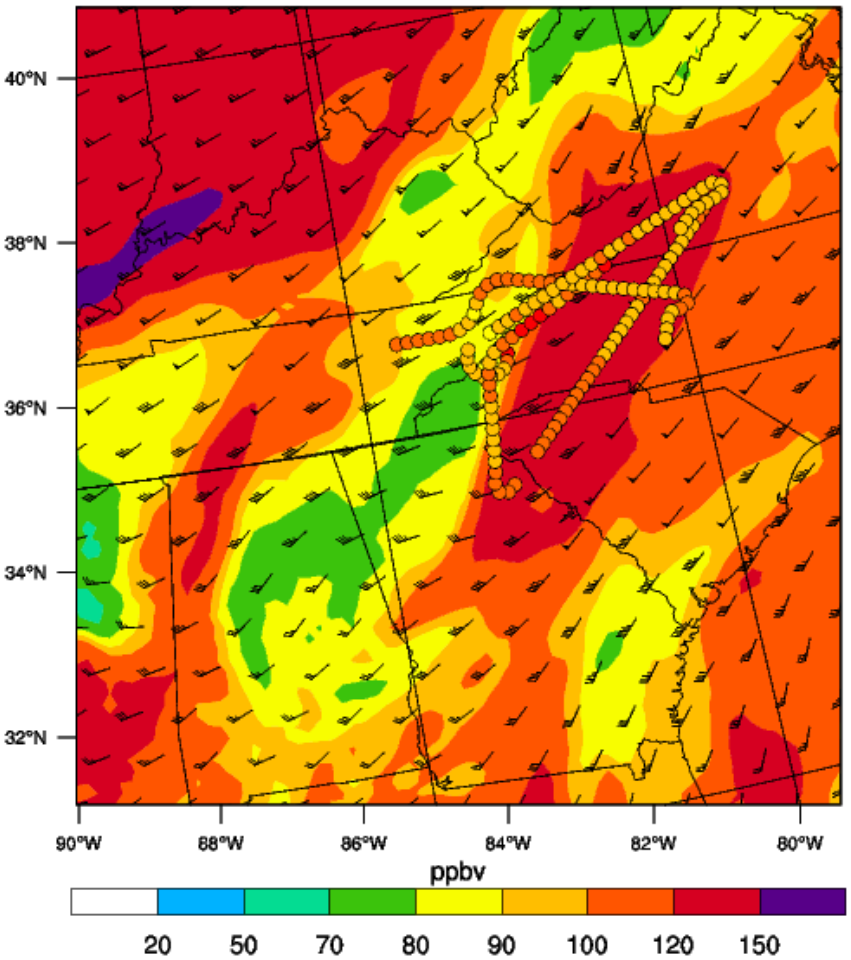
WRF-Chem O_3 values at 11km compare well with DC8 and GV observations in May 29 storm, but O_3 is overestimated in downwind flight sampling region

O_3 (ppbv) simulated by WRF-Chem at 11km and observed by DC8 and GV for 10<z<12km

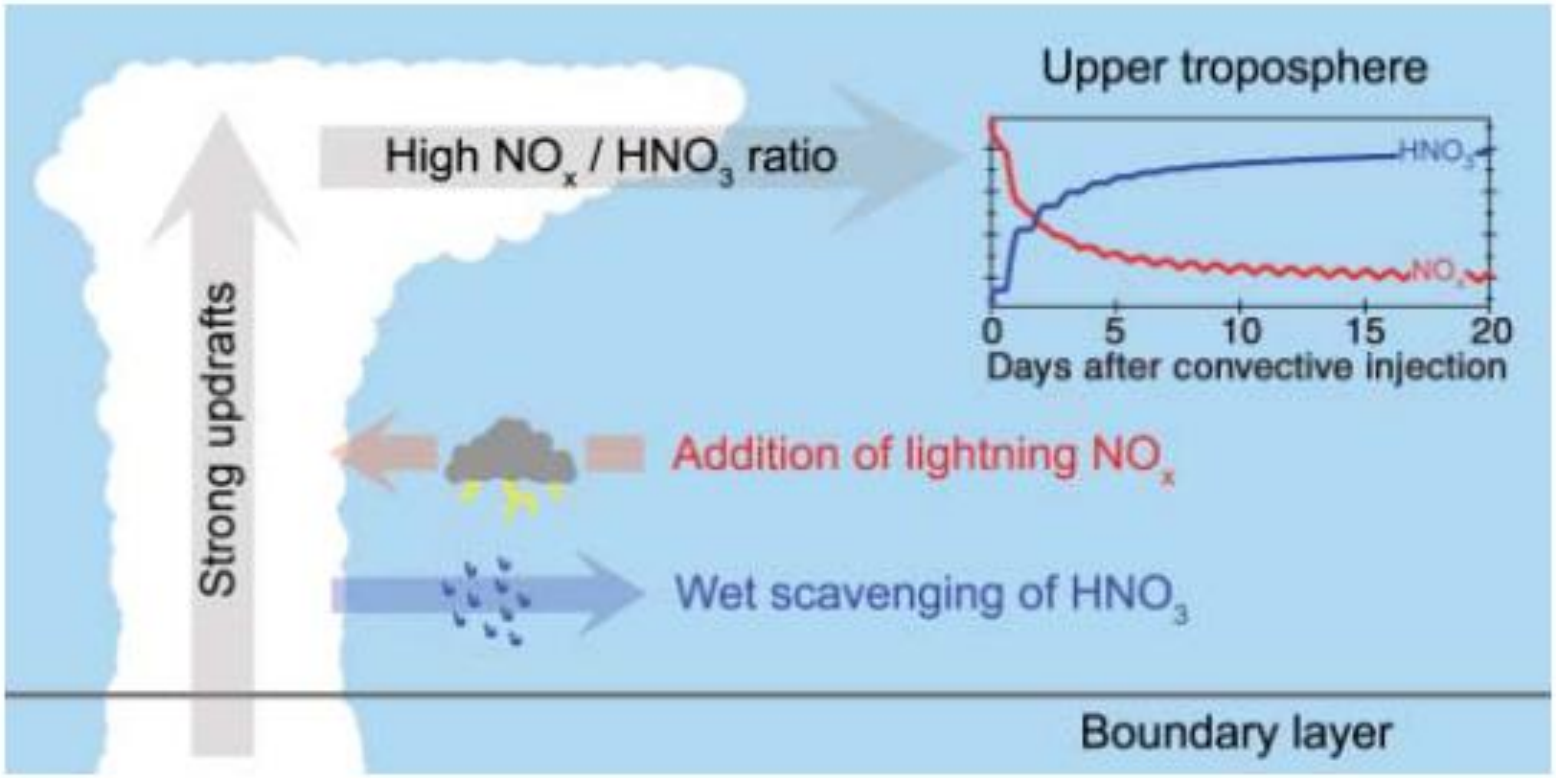
2012-05-30 0Z



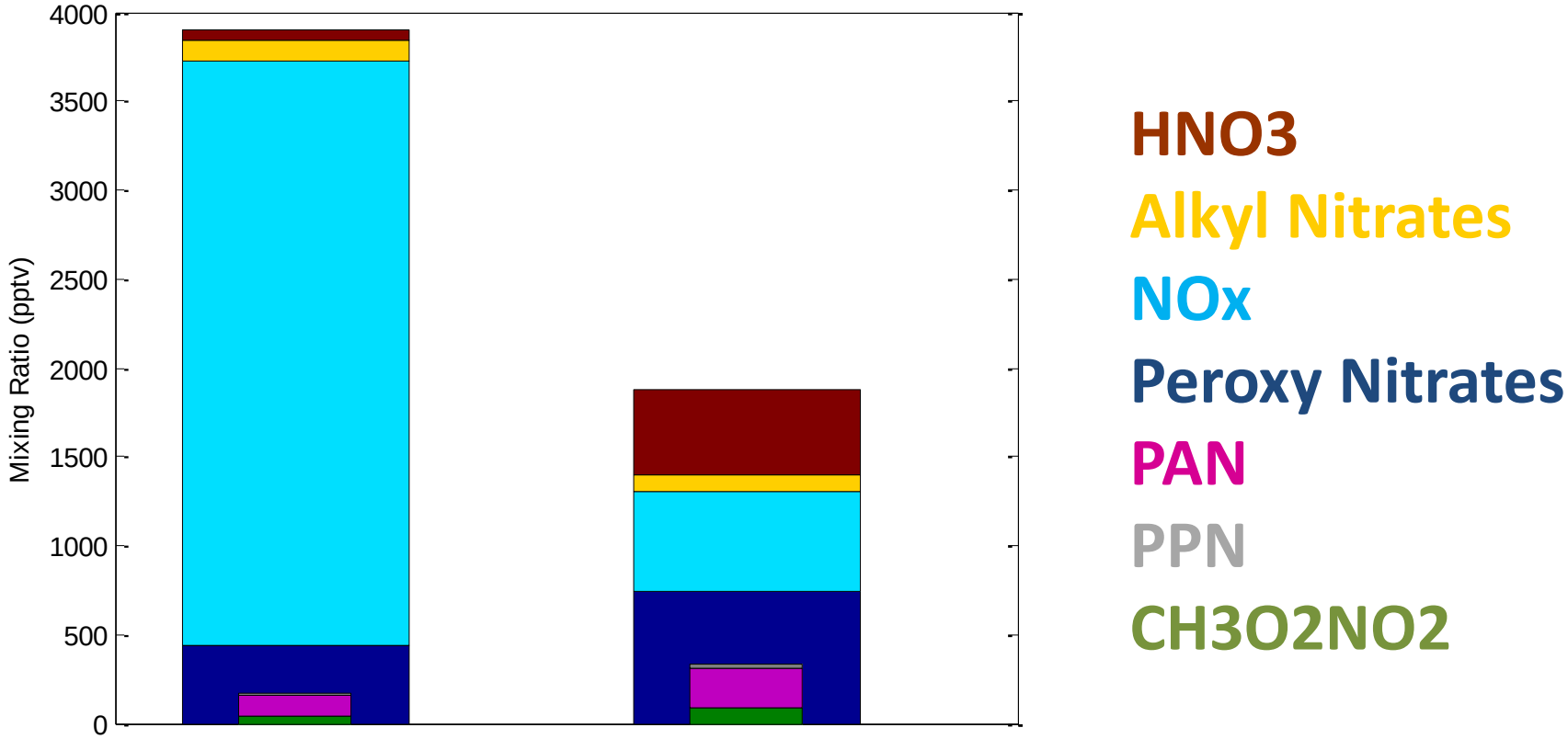
2012-05-30 22Z



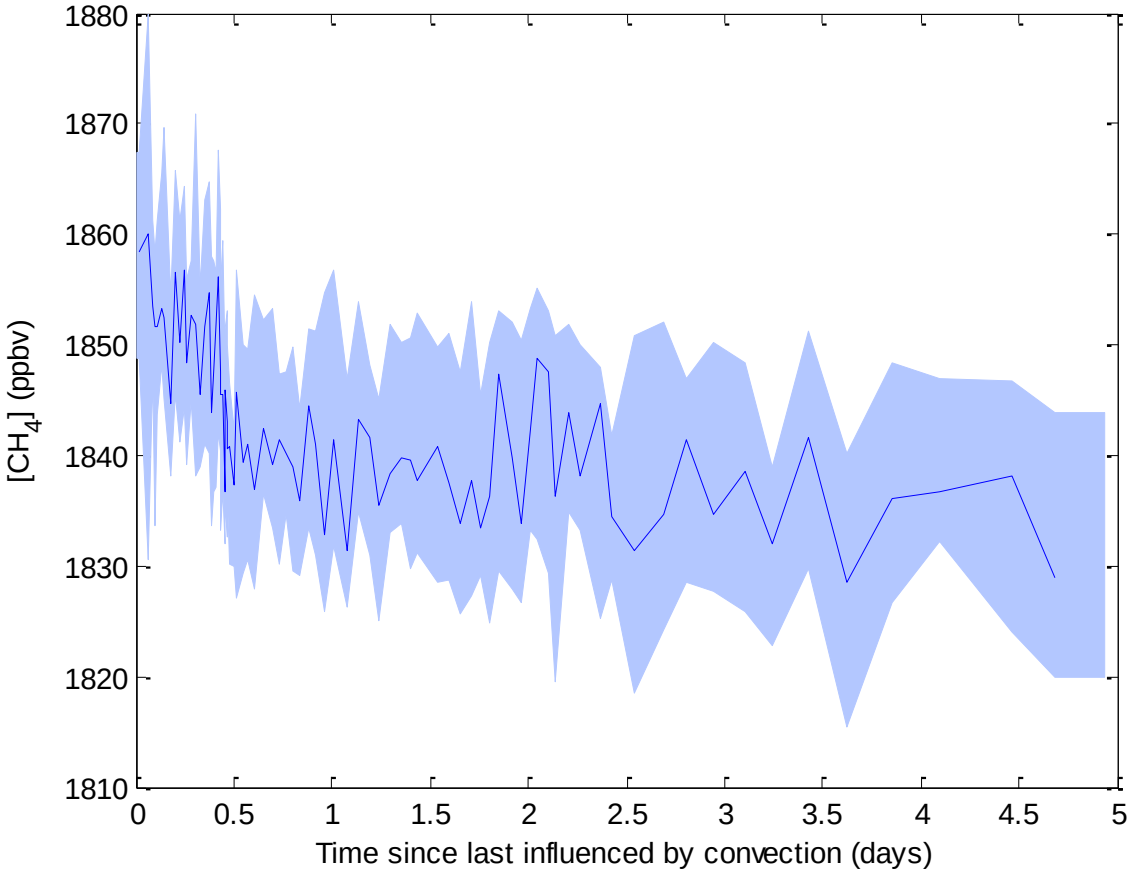
NO_x/HNO_3 Clock



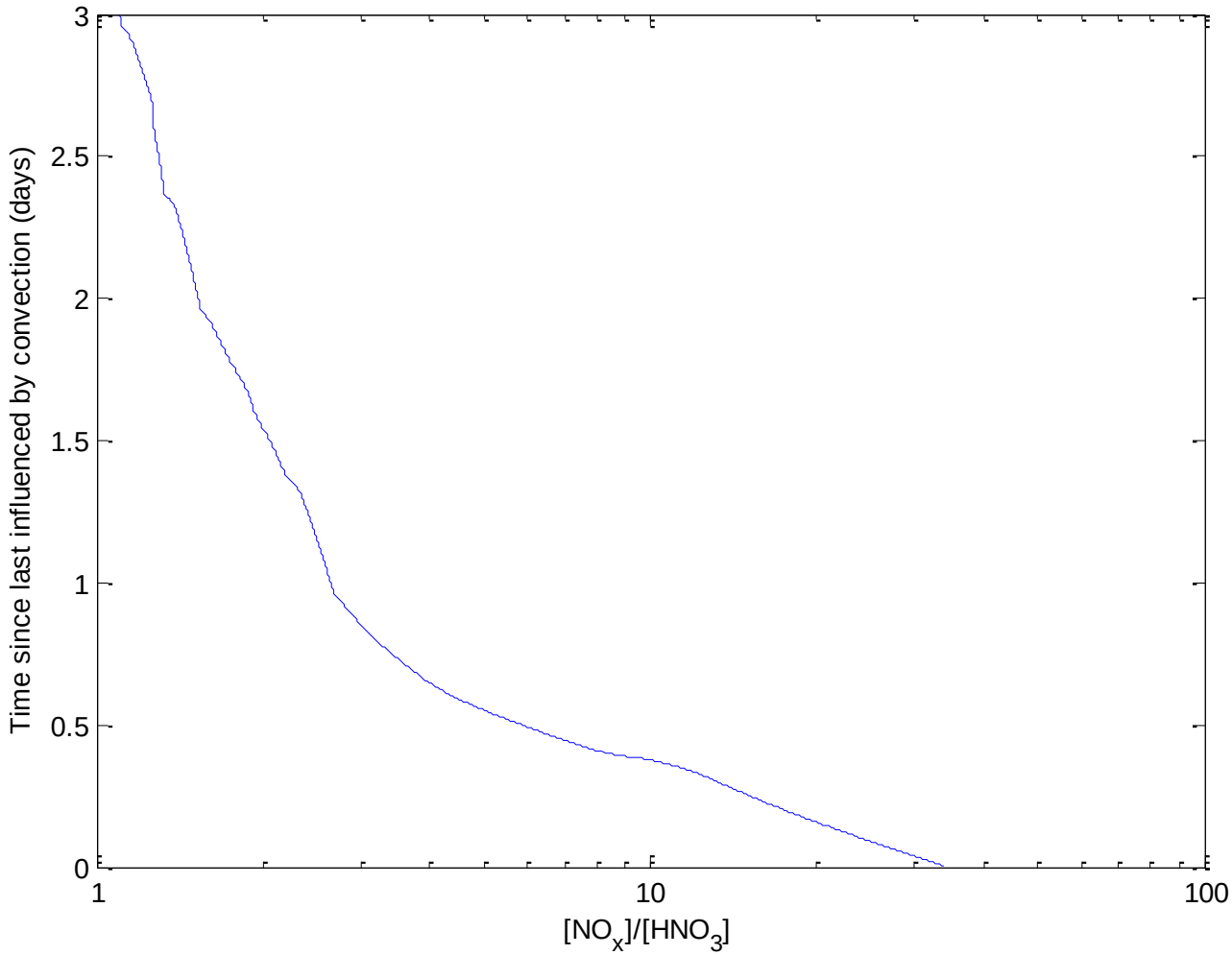
05/29 Average NO_y Budget vs. 05/30



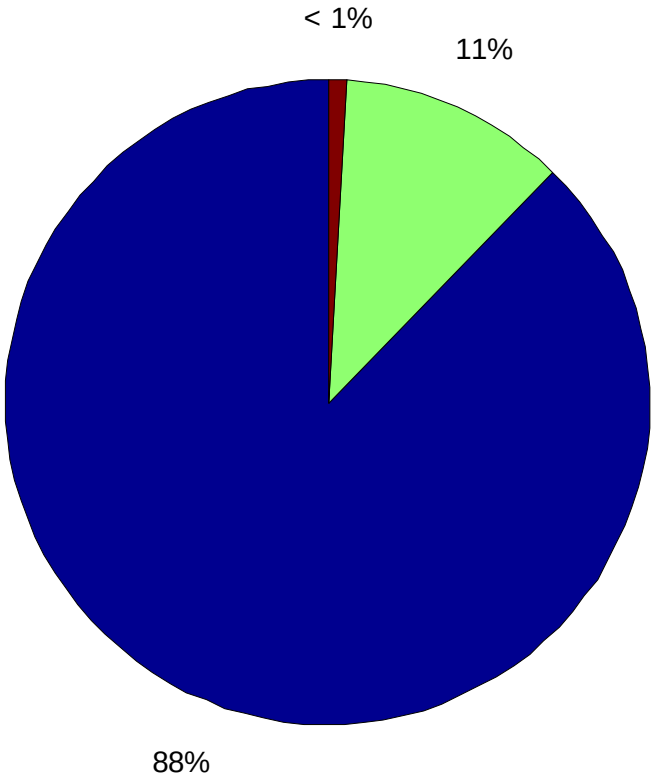
Role of Dilution



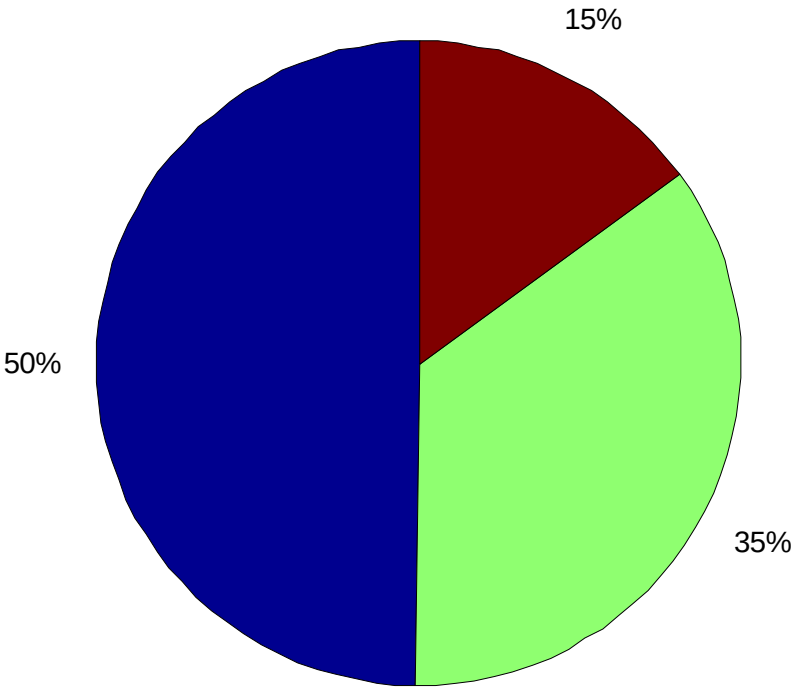
Example of NO_x/HNO_3 Clock



Evolution of NO_y Downwind from Convection

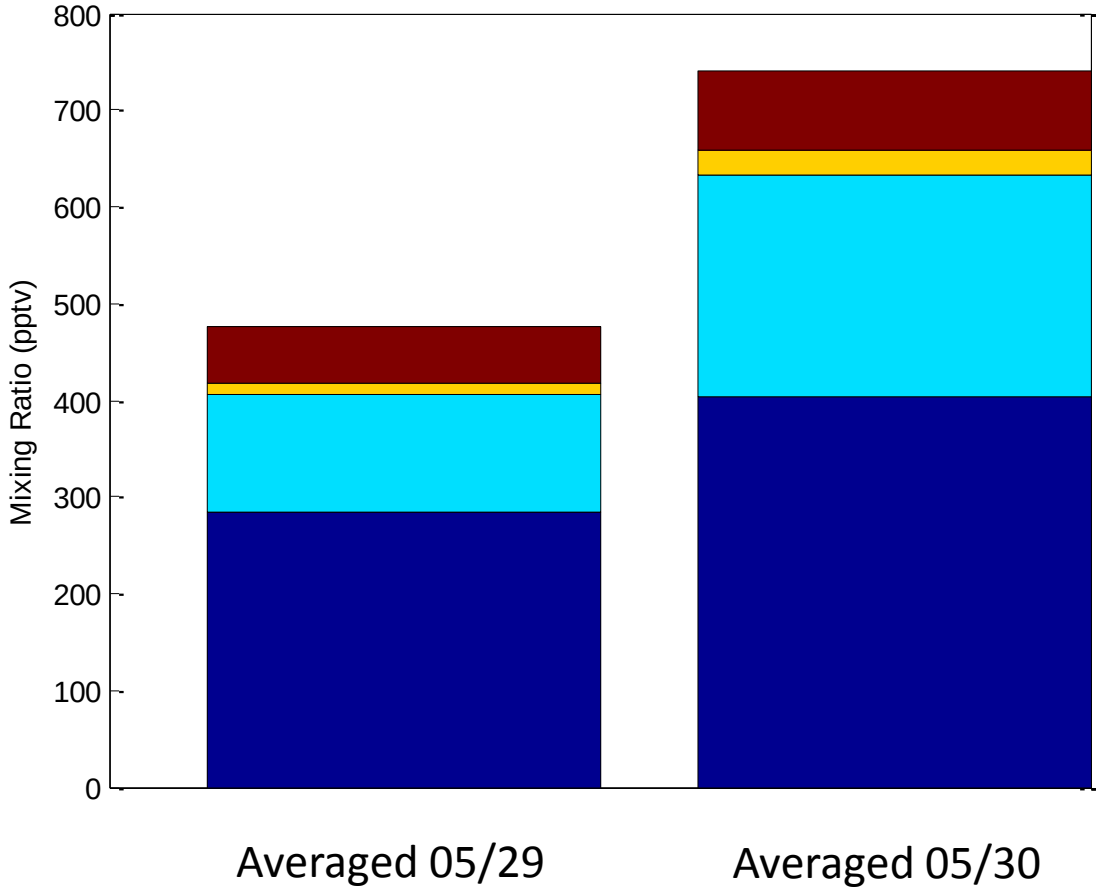


t=0 of Model



t=24 hrs of Model

How Do PNs Speciate



CH3O2NO2

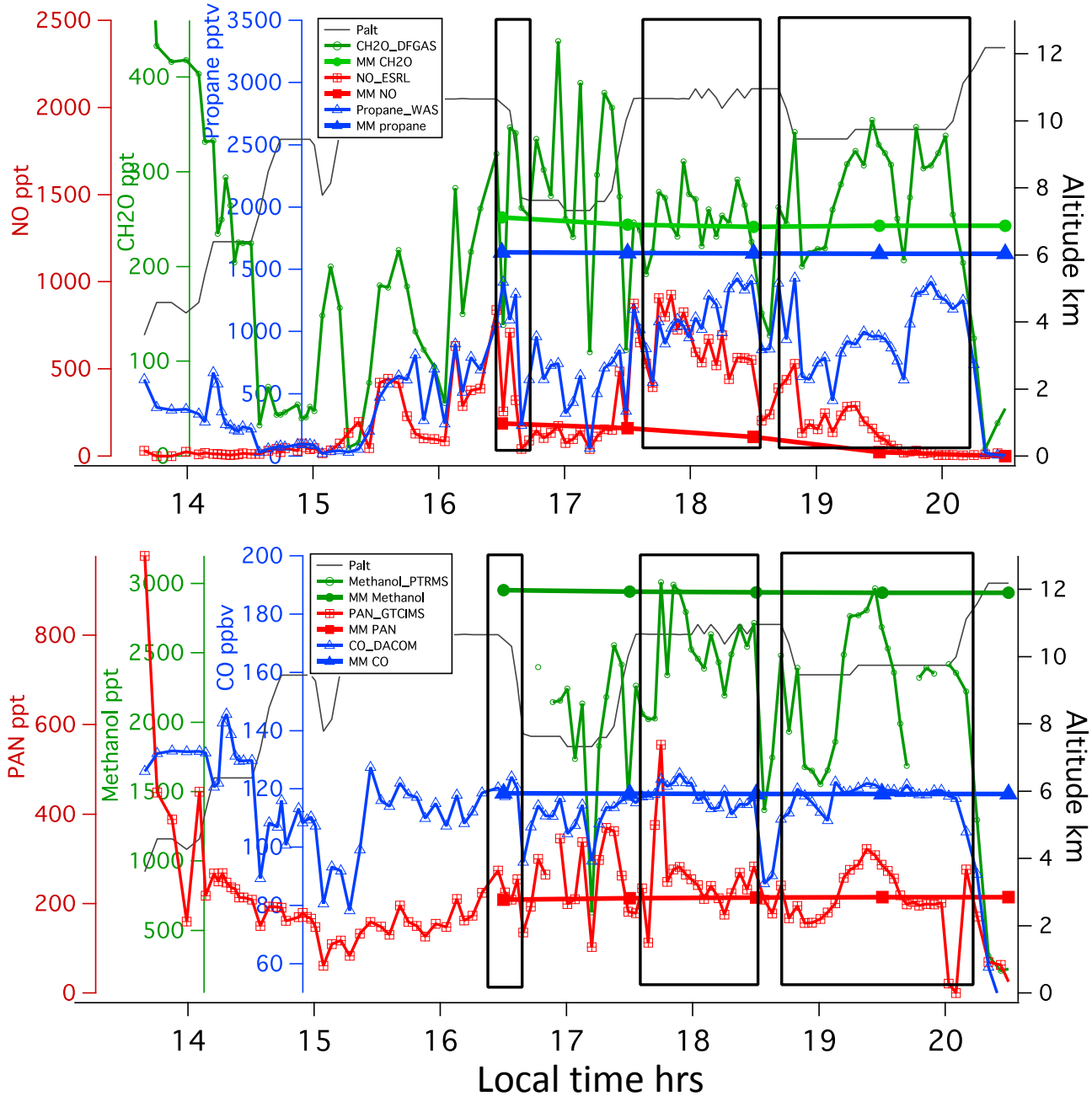
PPN

PAN

HO2NO2

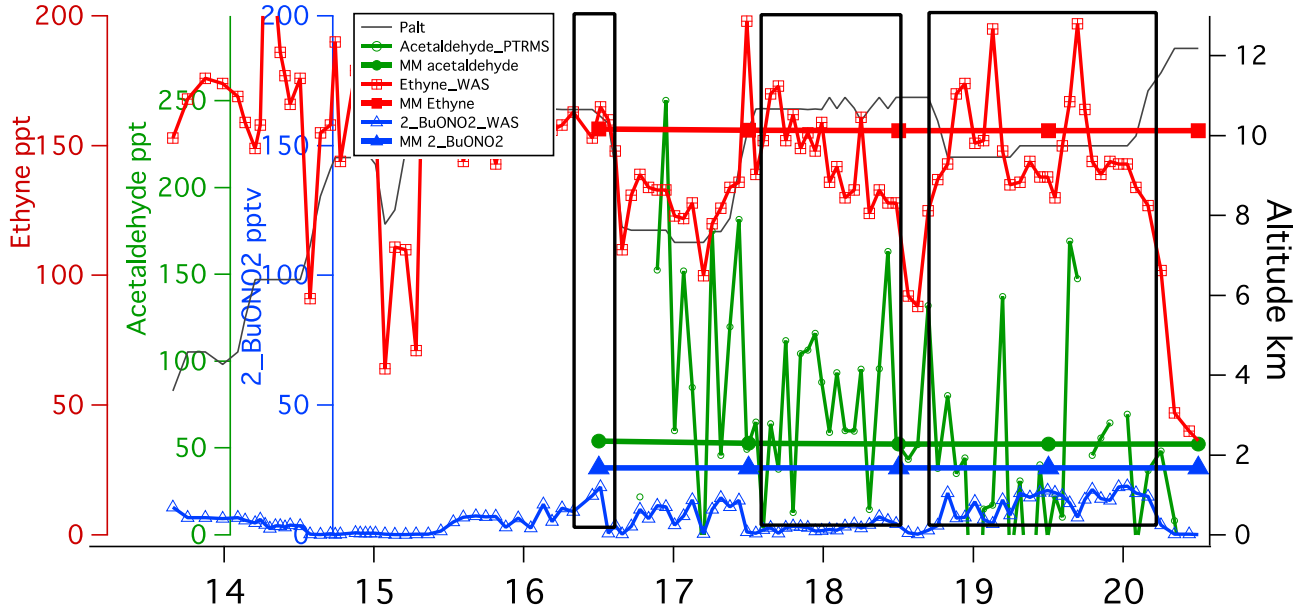
DC-3 "Day after" MM model results: May 29th outflow modeled and May 30th measurements

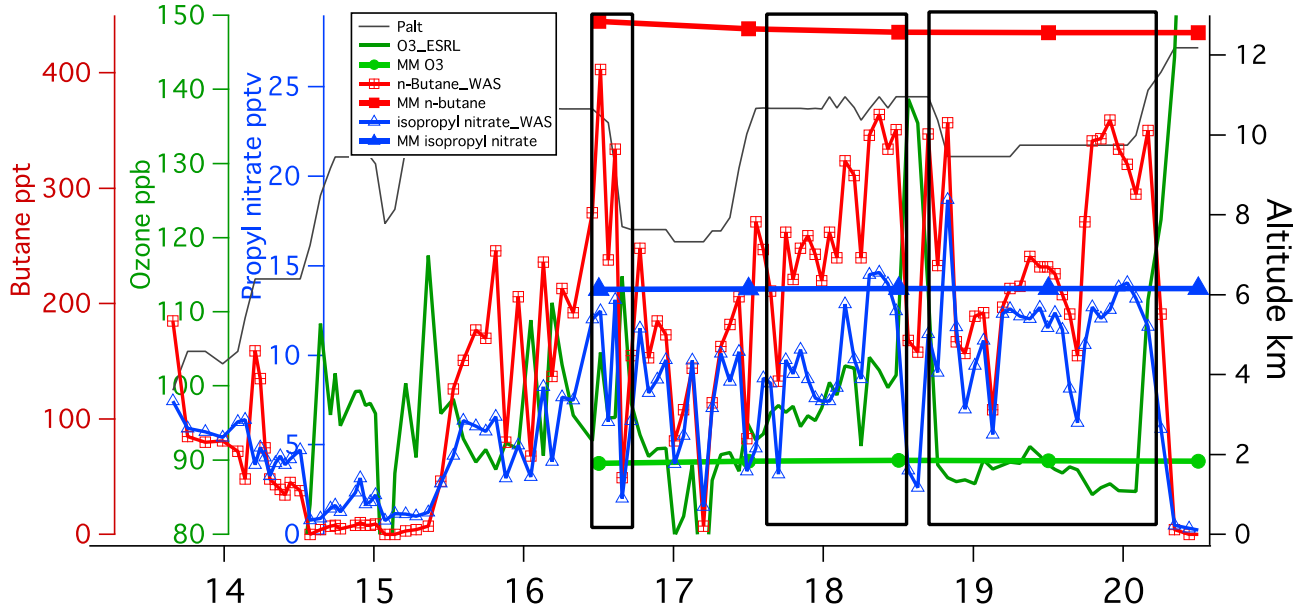
May 30th DC-8 : Boxed-in areas represent times where it is most probable that aged outflow from May 29 was being sampled.



DC-3 "Day after" MM model results: May 29th outflow modeled and May 30th measurements

May 30th DC-8 : Boxed-in areas represent times where it is most probable that aged outflow from May 29 was being sampled.



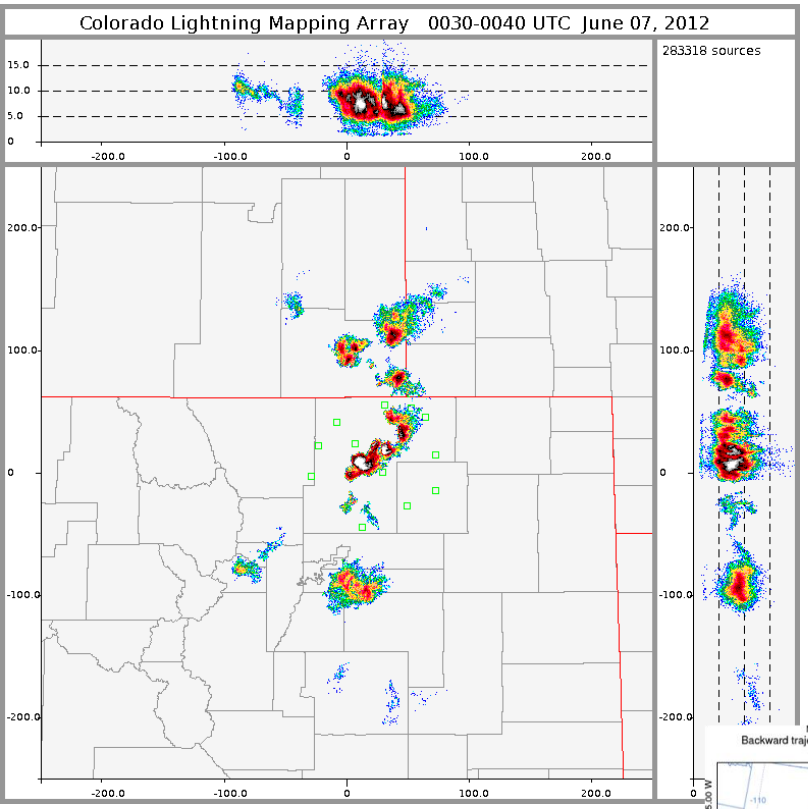


Local time hrs

June 7 Transport Downwind of June 6 Colorado Convection

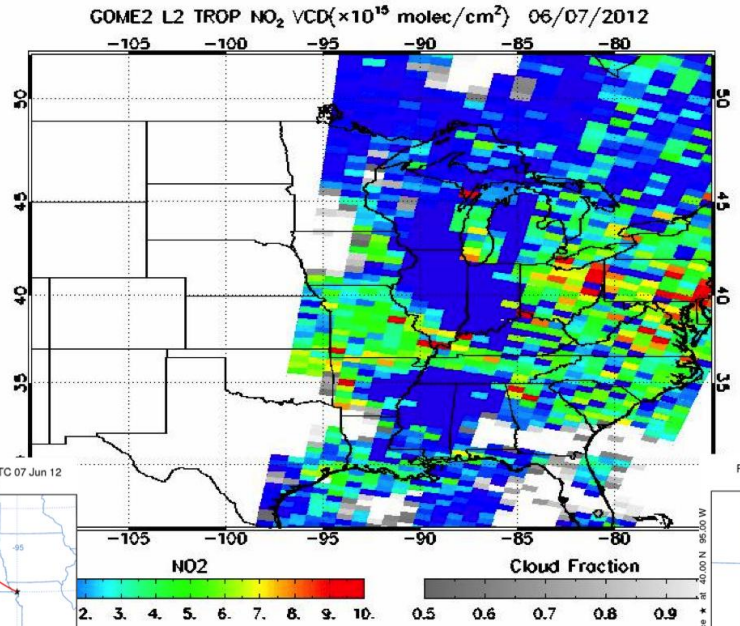
Kristin Cummings, Ken Pickering, Megan Bela, Mary Barth

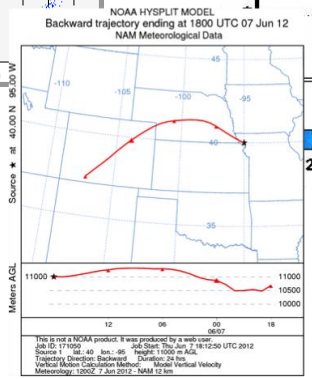
June 6 Colorado Storms

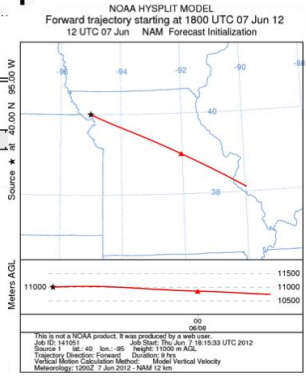


Chemical evolution of outflow to be simulated with WRF-Chem run at 3-km resolution for Colorado storms nested in 15-km domain extending eastward to beyond Illinois

GOME NO2 Imagery **June 7**





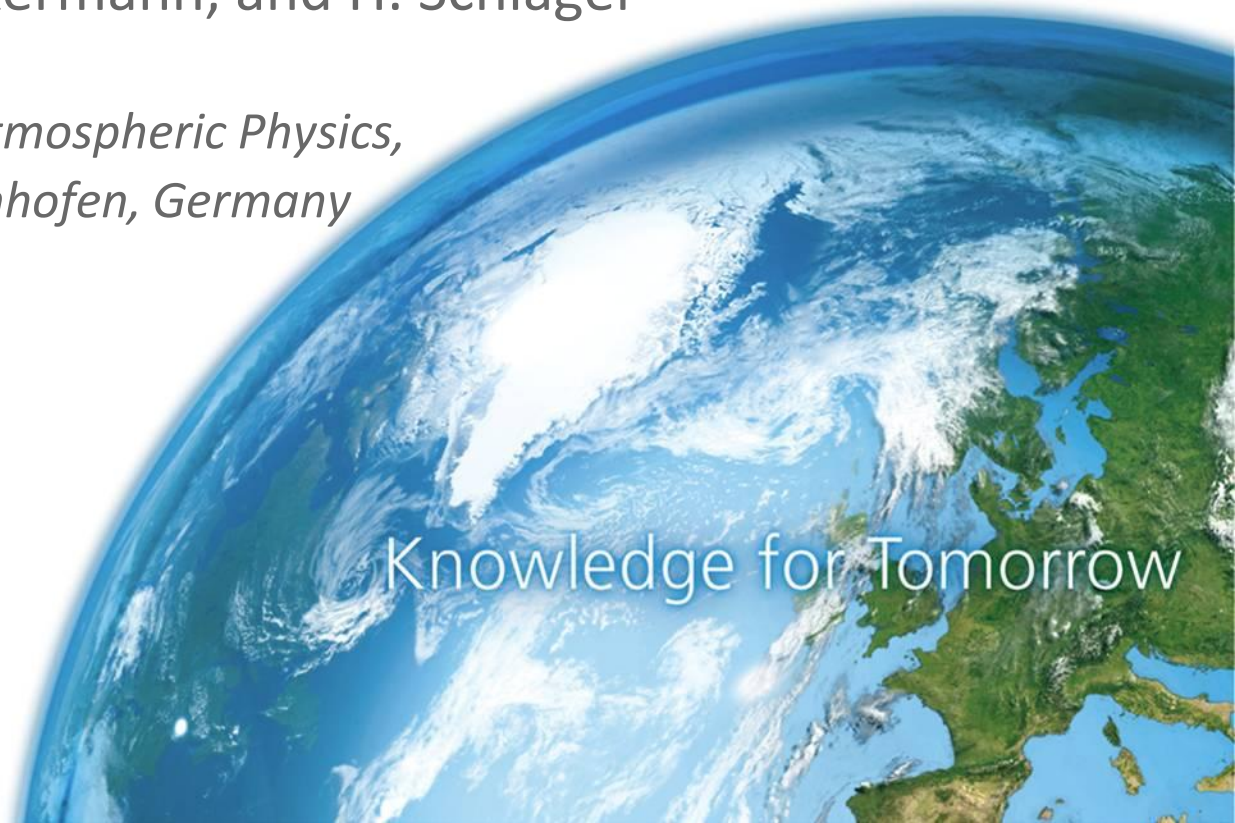


HYSPLIT trajectories show high NOx in northwest Missouri came from Colorado at 00z previous evening. This air then travels to southeast Missouri.

Some DC3 Highlights - aged LNOx - from the Perspective of the German DLR Falcon Aircraft

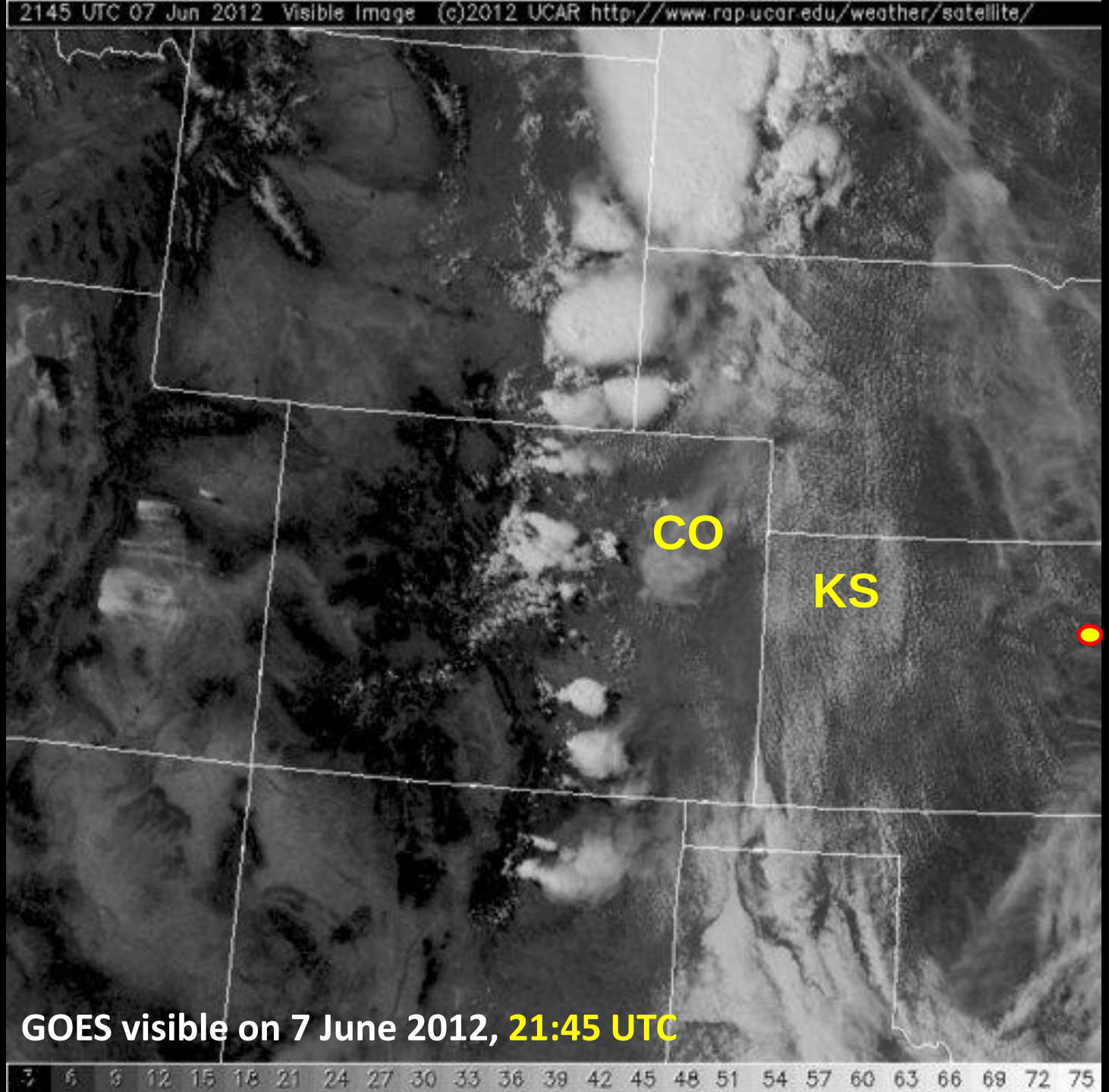
H. Huntrieser*, M. Lichtenstern, A. Minikin, T. Pucik, M. Scheibe, H. Aufmhoff, A. Roiger, B. Rappenglück, L. Ackermann, and H. Schlager

**DLR - Institute of Atmospheric Physics, Oberpfaffenhofen, Germany*

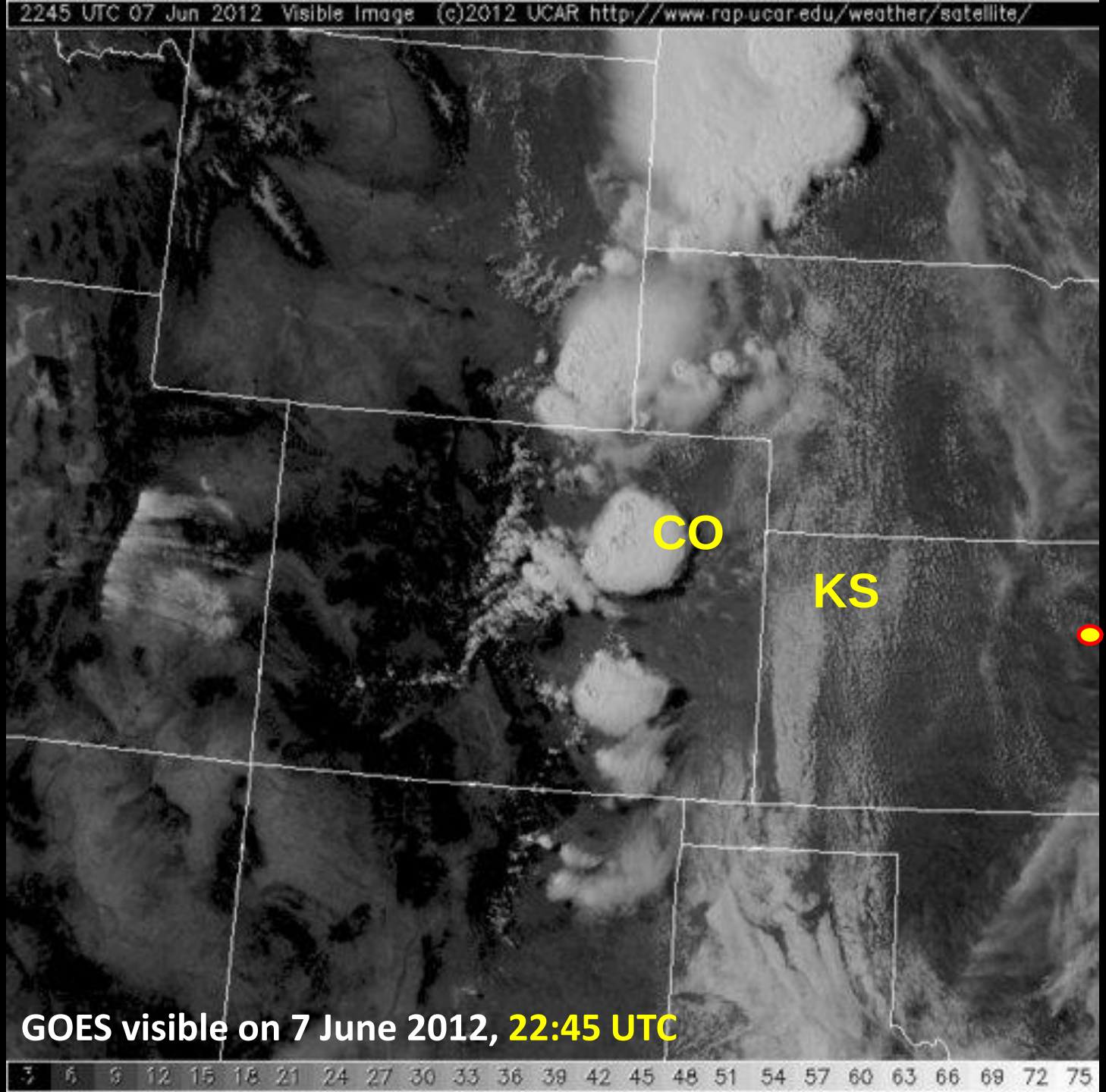


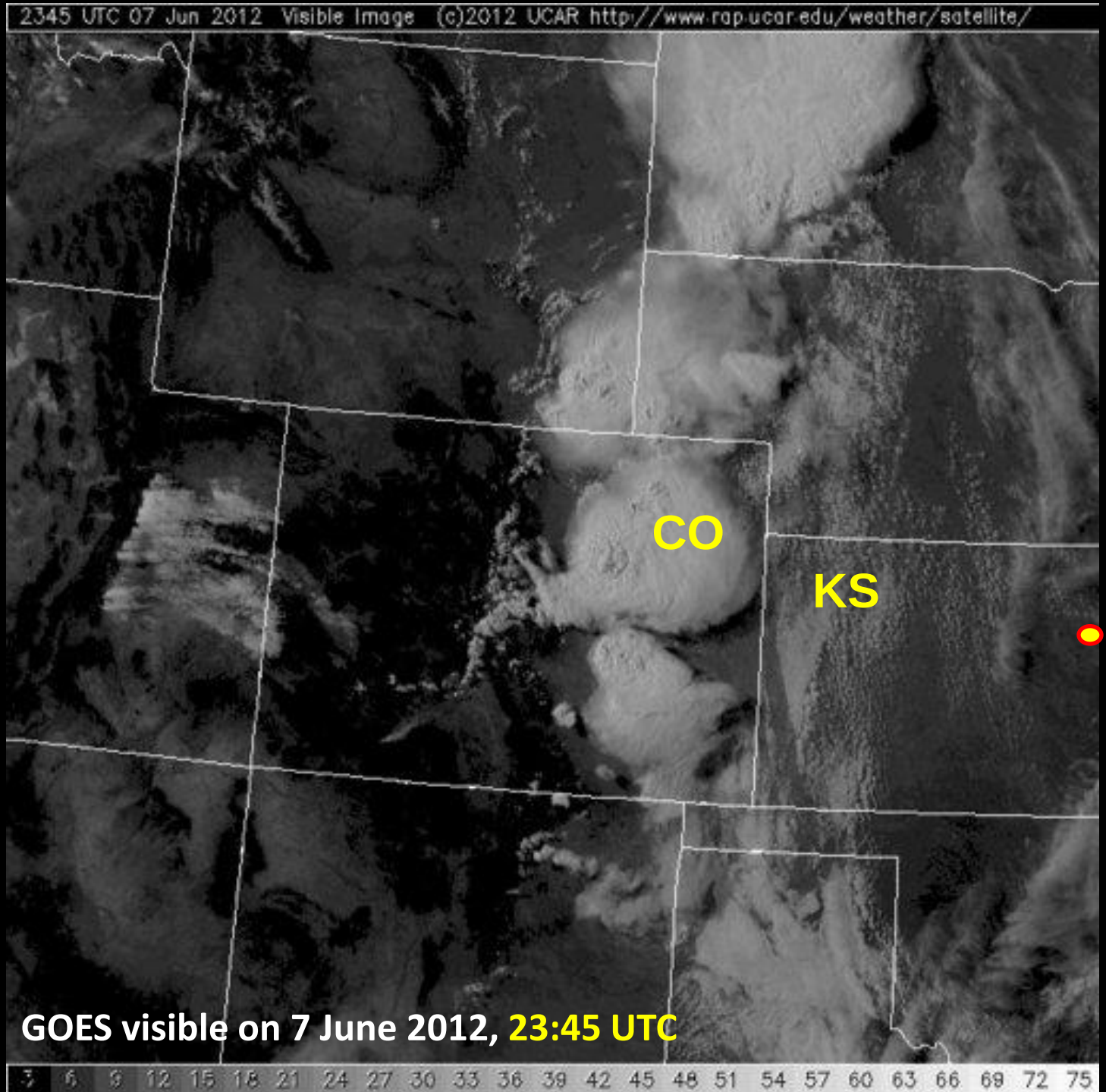
DLR
Deutsches Zentrum für Luft- und Raumfahrt

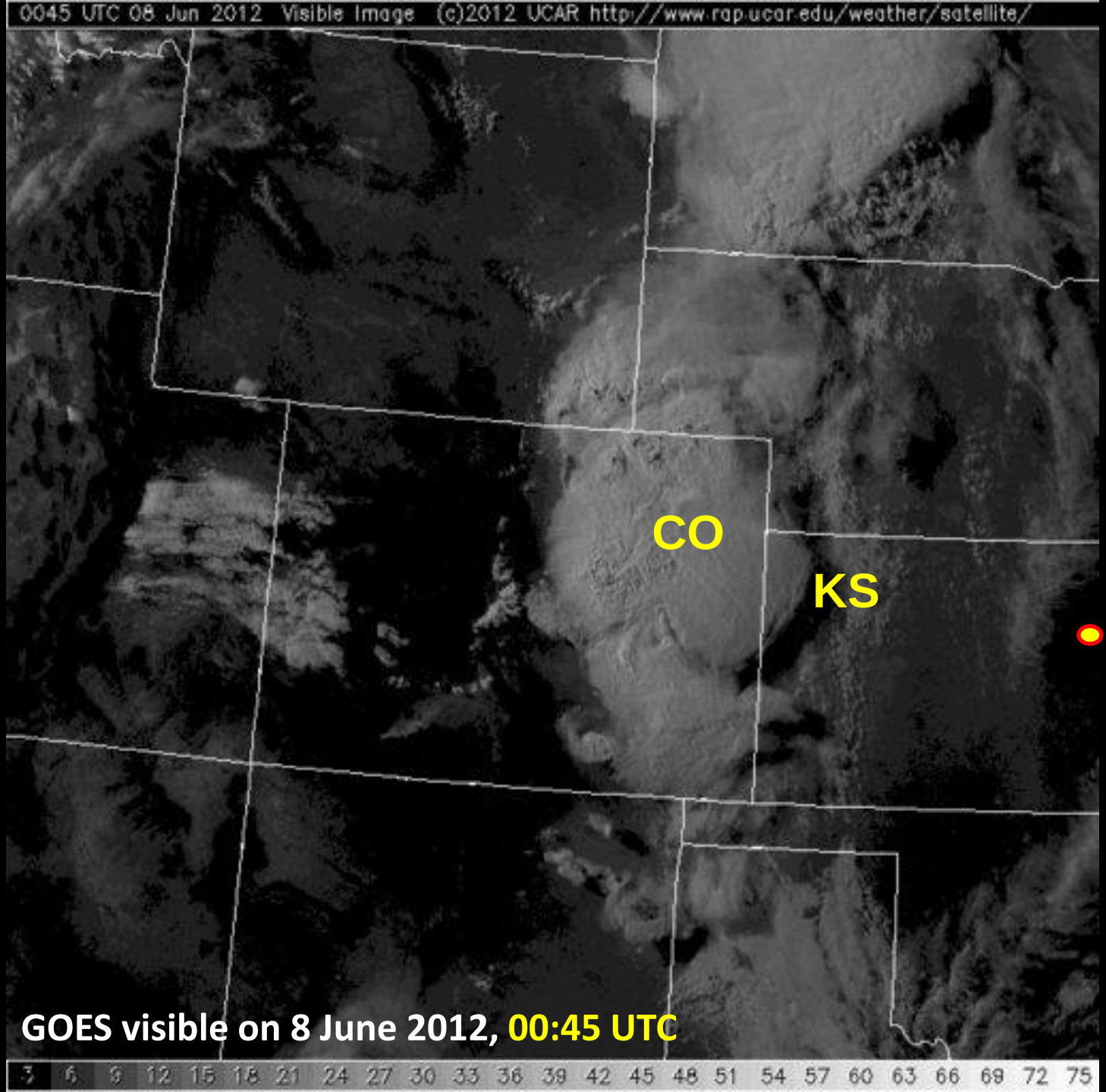
Date 2012	Aged LNOx (CO)	BB Whitewater-Baldy (NM)	BB Little Bear (NM)	BB High Park (CO)	BB Canada	Aged LNOx (OK/TX)	Asian-CO
29 May (2x)		**X** (no CO, 80 O3)					
30 May (2x)		**X** (500 CO, 80 O3)					
5 June (2x)	**(X)** (110 CO, 80-100 O3)						
6 June (flash)							
8 June (2x)	**X** (**1 NO**, 110 CO, 80-110 O3)					**X** (150 CO, 100 O3)	
11 June (2x)			**X** (700 CO, 80 O3)	**X** (130 CO, 60 O3)	**(X)**		
12 June			**(X)**	**X** (140 CO, 60 O3)			**X** (160 CO, 120 O3)
14 June				**X** (130 CO, 90 O3)			



GOES visible on 7 June 2012, 21:45 UTC


2245 UTC 07 Jun 2012 Visible Image (c)2012 UCAR http://www.rap.ucar.edu/weather/satellite/
CO
KS
Salina
GOES visible on 7 June 2012, 22:45 UTC
3 6 9 12 15 18 21 24 27 30 33 36 39 42 45 48 51 54 57 60 63 66 69 72 75


2345 UTC 07 Jun 2012 Visible Image (c)2012 UCAR http://www.rap.ucar.edu/weather/satellite/
CO
KS
Salina
GOES visible on 7 June 2012, 23:45 UTC
3 6 9 12 15 18 21 24 27 30 33 36 39 42 45 48 51 54 57 60 63 66 69 72 75

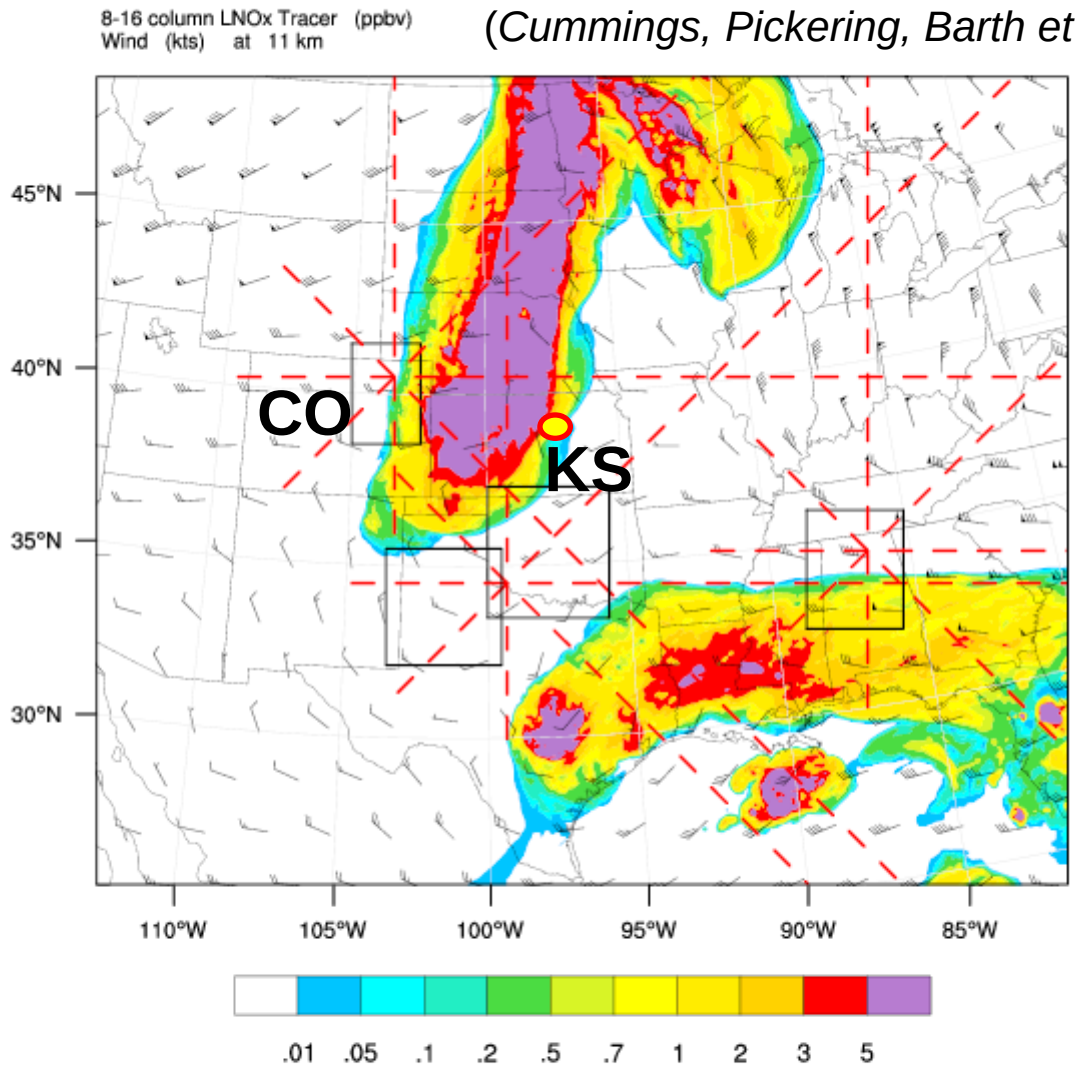

0045 UTC 08 Jun 2012 Visible Image (c)2012 UCAR http://www.rap.ucar.edu/weather/satellite/
CO
KS
Salina
GOES visible on 8 June 2012, 00:45 UTC
3 6 9 12 15 18 21 24 27 30 33 36 39 42 45 48 51 54 57 60 63 66 69 72 75

2012-06-08_11:00:00

NCAR WRF ARW Forecast (Δx=3 km)

8-16 km column LNOx Tracer (ppbv)

(*Cummings, Pickering, Barth et al.*)



NCAR WRF ARW Forecast (Δx=3 km)

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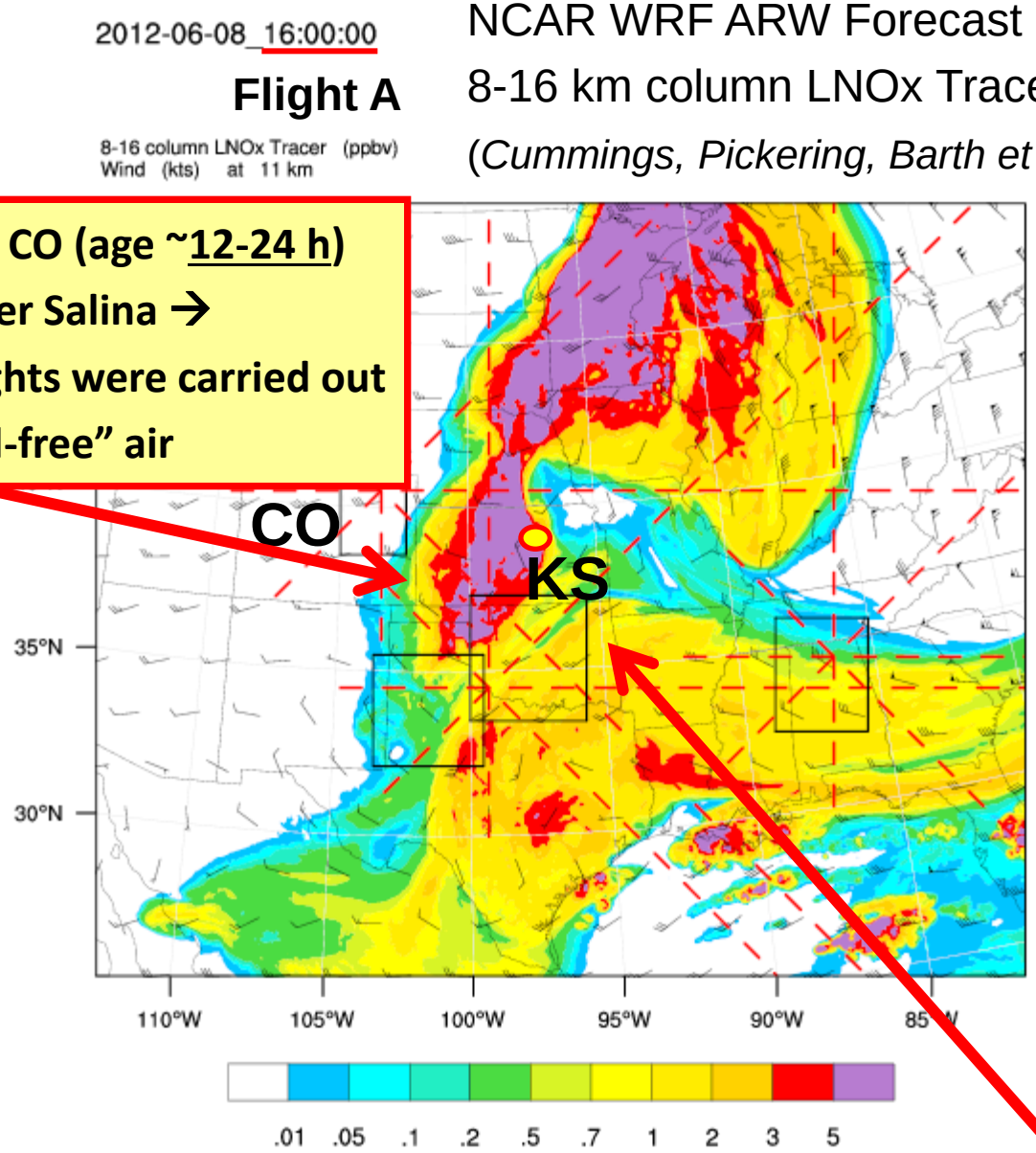
(*Cummings, Pickering, Barth et al.*)



LNOx plume from CO (age ~12-24 h) directly over Salina →

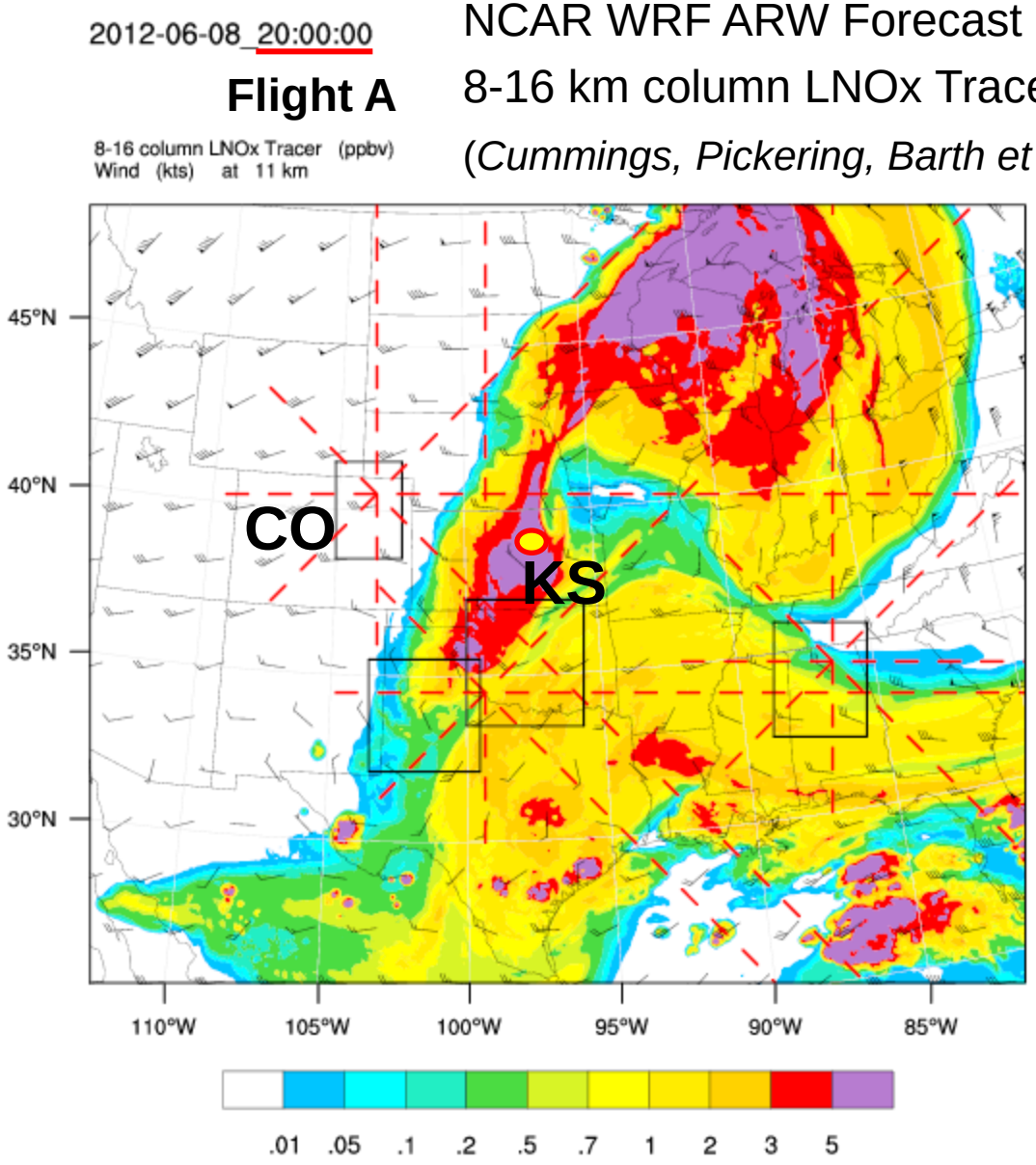
2 Falcon mission flights were carried out in "cloud-free" air

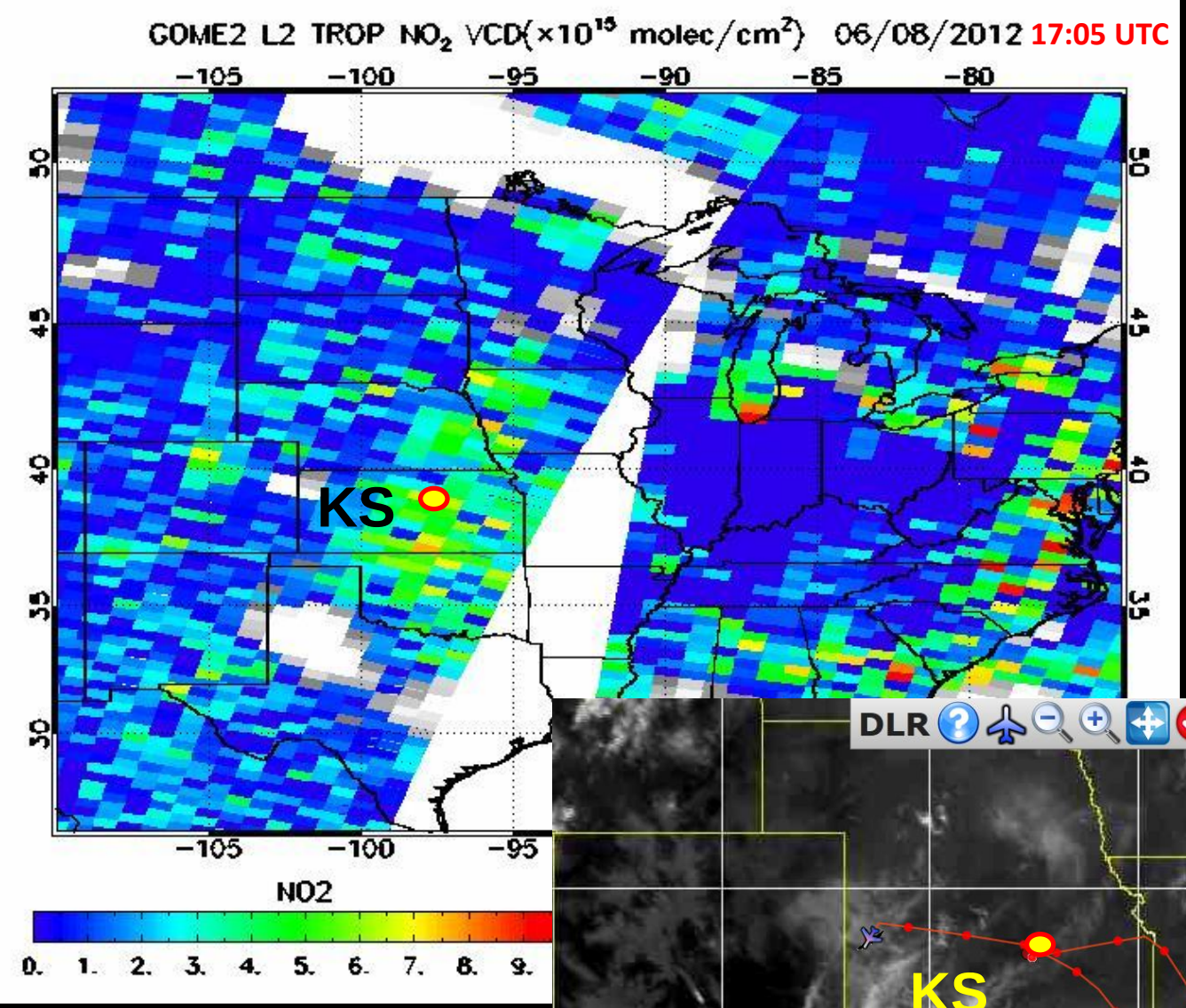
LNOx plume from OK/TX (age ~24-48 h) over SE Kansas

NCAR WRF ARW Forecast (Δx=3 km)

8-16 km column LNOx Tracer (ppbv)

(*Cummings, Pickering, Barth et al.*)

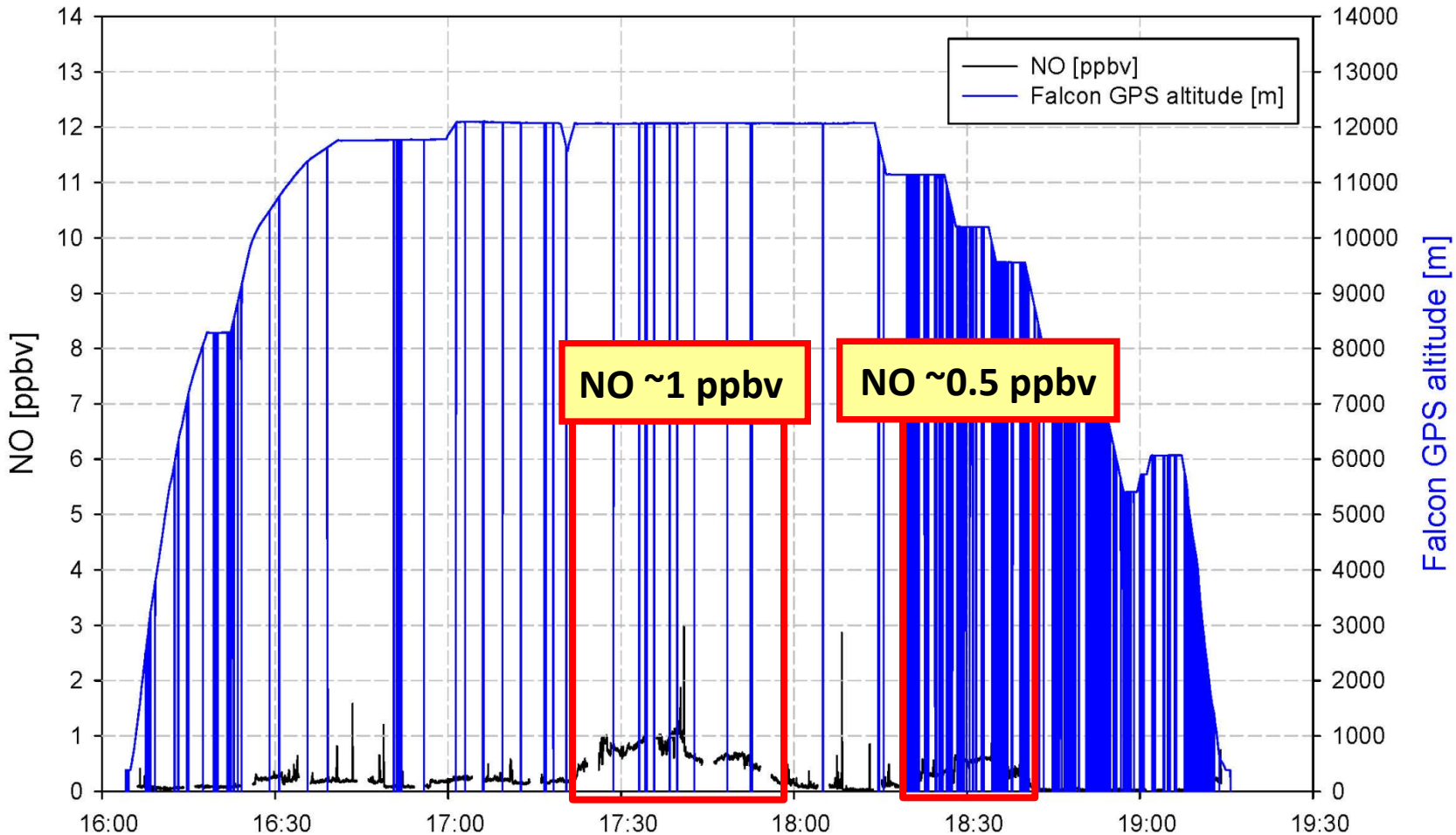



GOME2 L2 TROP NO_2 VCD($\times 10^{15}$ molec/cm^2) 06/08/2012 17:05 UTC
−105 −100 −95 −90 −85 −80
50 45 40 35 30
KS
−105 −100 −95
NO2
0. 1. 2. 3. 4. 5. 6. 7. 8. 9.

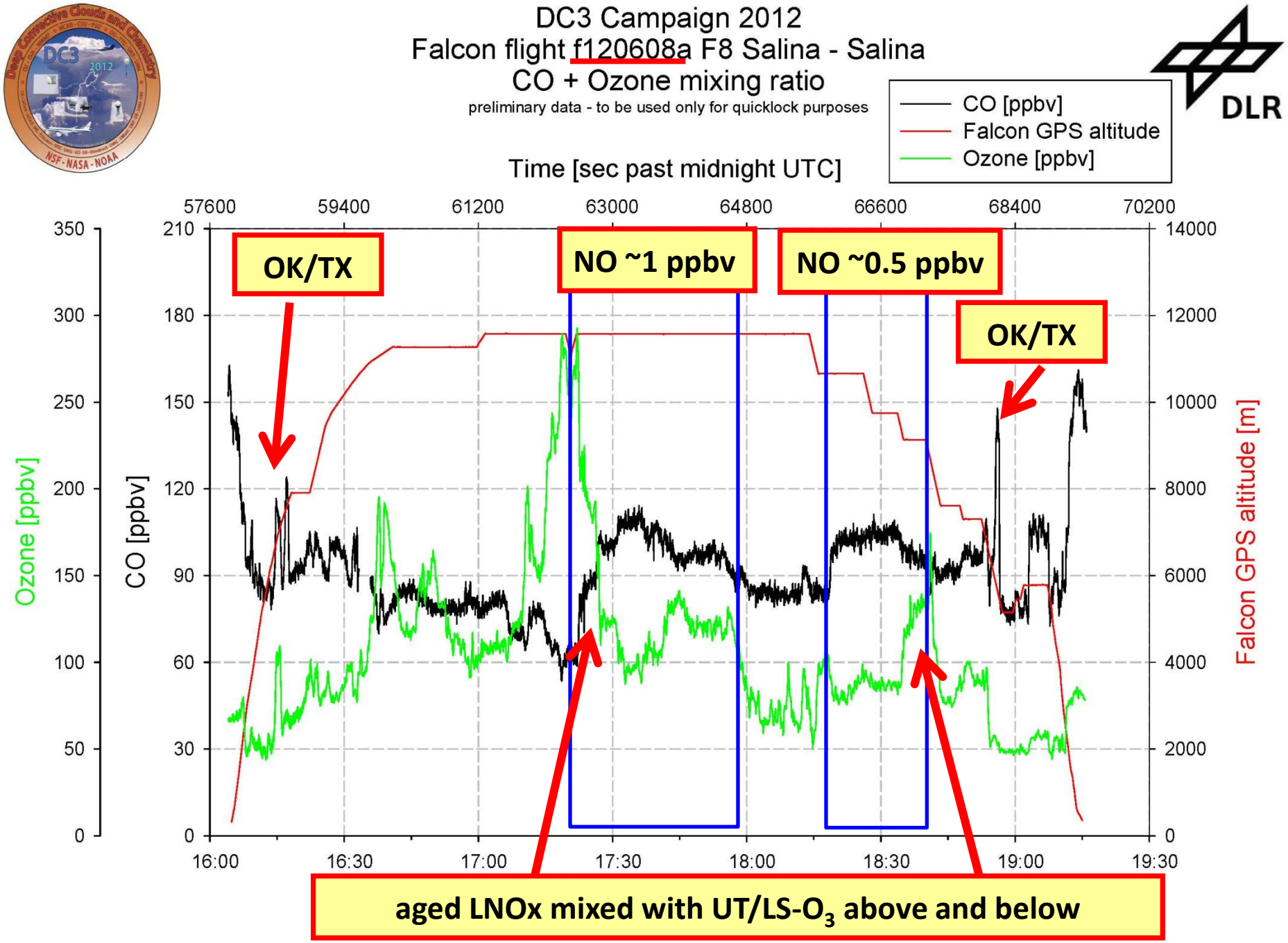
DLR
KS
06/08/2012 1739 UTC GOES-13 IR Ch4
06/08/2012 1739 UTC GOES-13 VIS Ch1

DC3 Campaign 2012
Falcon flight f120608a F8 Salina - Salina
NO mixing ratio

preliminary data - to be used only for quicklock purposes



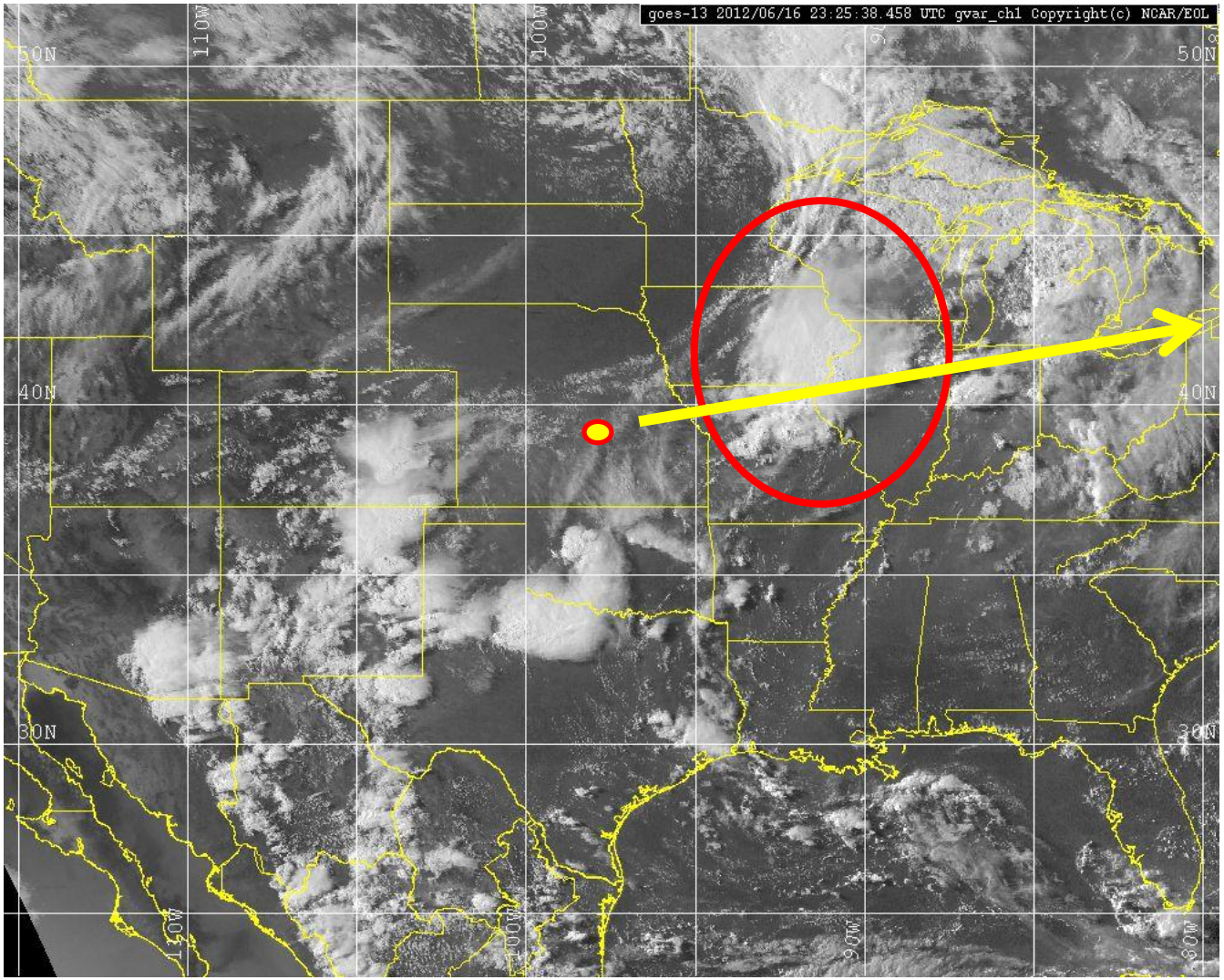
aged LNOx probed above ~9 km (up to 12 km) for ~1 h during each of the 2 flights


DC3 Campaign 2012
Falcon flight f120608a F8 Salina - Salina
CO + Ozone mixing ratio
preliminary data - to be used only for quicklock purposes
CO [ppbv]
Falcon GPS altitude
Ozone [ppbv]
Time [sec past midnight UTC]
57600
59400
61200
63000
64800
66600
68400
70200
Ozone [ppbv]
CO [ppbv]
Falcon GPS altitude [m]
16:00
16:30
17:00
17:30
18:00
18:30
19:00
19:30
OK/TX
NO ~1 ppbv
NO ~0.5 ppbv
OK/TX
aged LNOx mixed with UT/LS-O3 above and below
DLR

Falcon transfer flight: 17 June 2012 from Salina to Syracuse

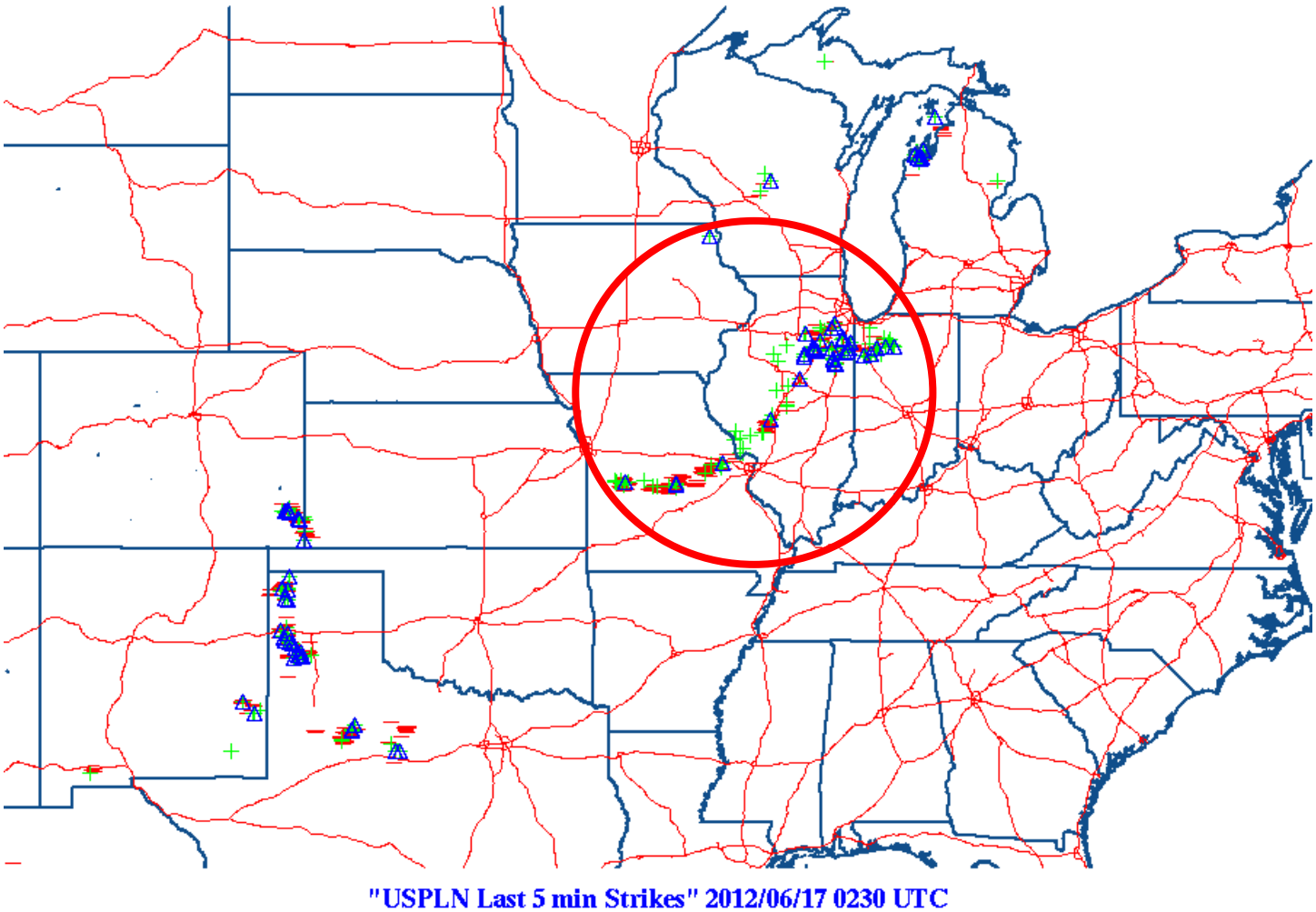
Penetration of a wide, aged LNOx area

Falcon transfer flight: 17 June 2012 from Salina to Syracuse



Cold front passage with convection the evening before the flight southwest of the Great Lakes

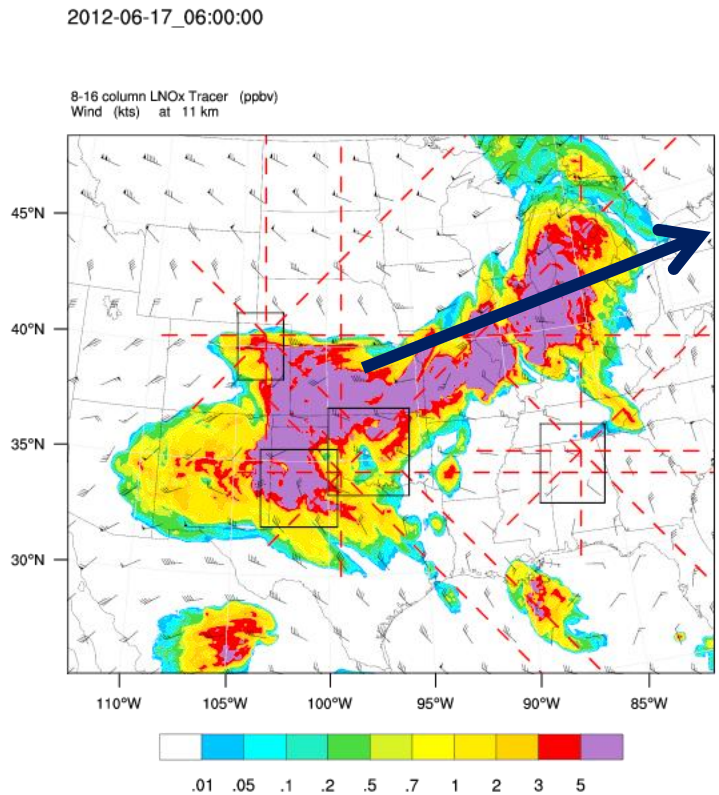
Falcon transfer flight: 17 June 2012 from Salina to Syracuse



Cold front passage with convection the evening before the flight southwest of the Great Lakes

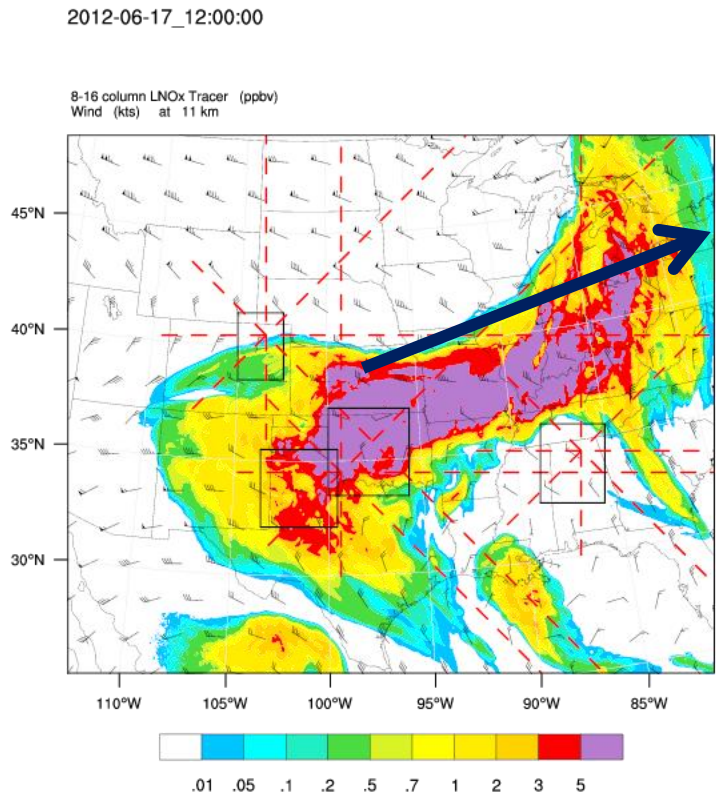
Falcon transfer flight: 17 June 2012 from Salina to Syracuse

Penetration of wide LNOx area



Falcon transfer flight: 17 June 2012 from Salina to Syracuse

Penetration of wide LNOx area

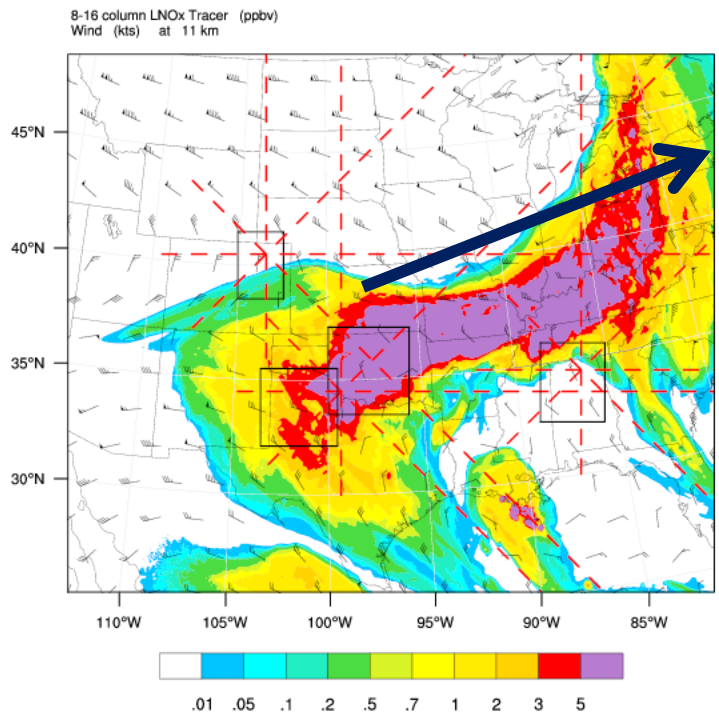


Falcon transfer flight: 17 June 2012 from Salina to Syracuse

Penetration of wide LNOx area

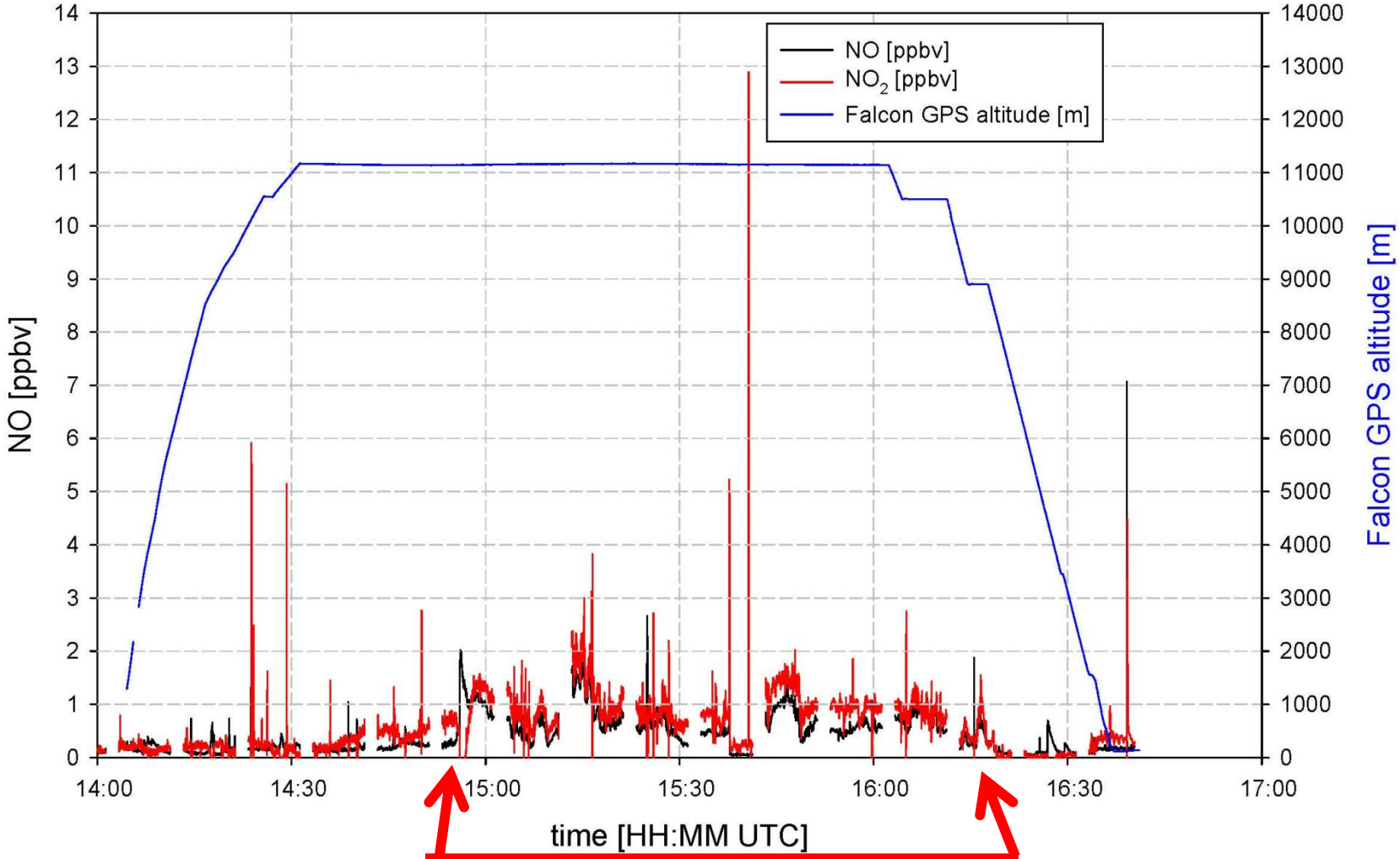
Time of the flight

2012-06-17_15:00:00

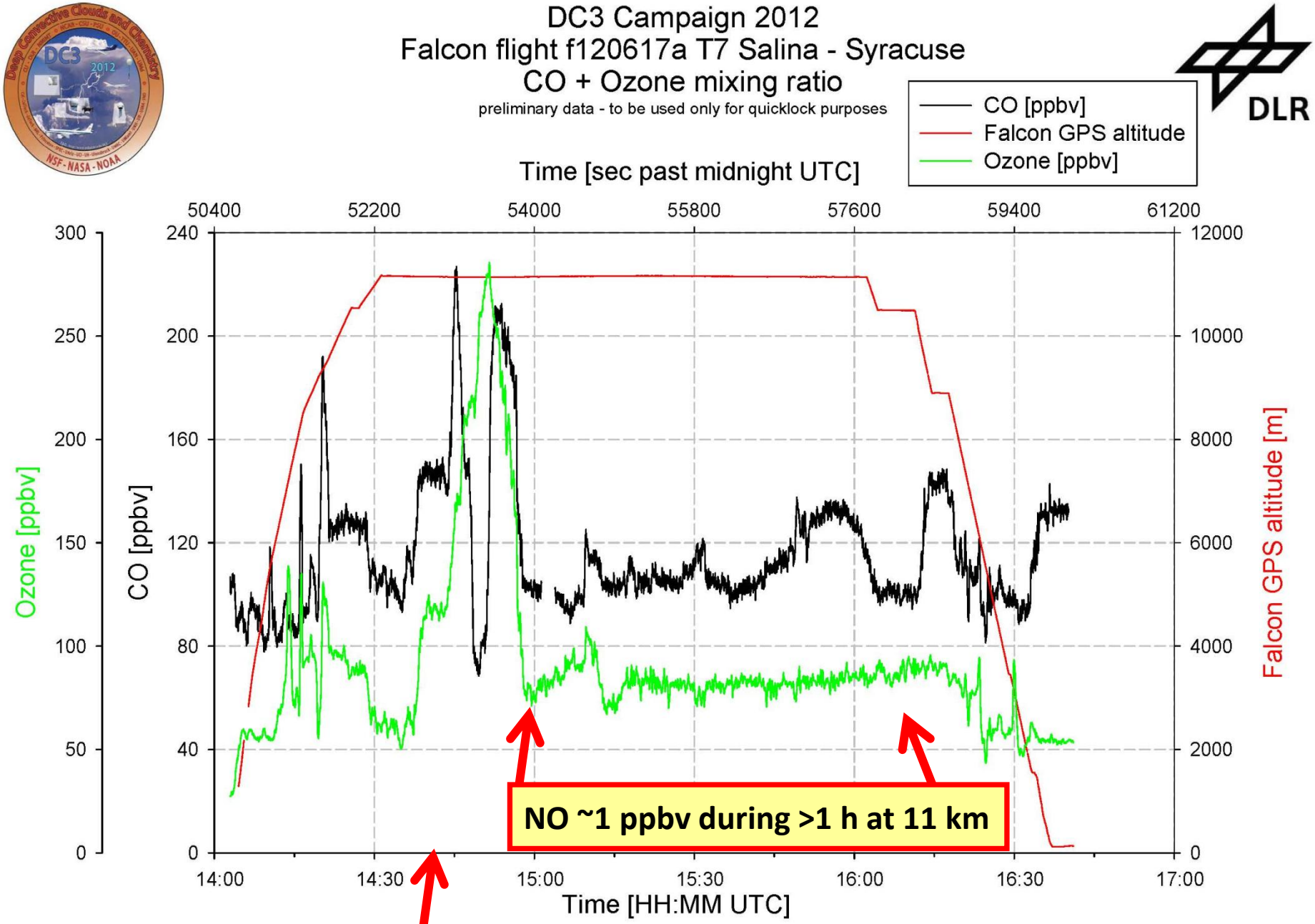


DC3 Campaign 2012
Falcon flight f120617a T7 Salina - Syracuse
NO + NO_2 mixing ratio

preliminary data - to be used only for quicklock purposes

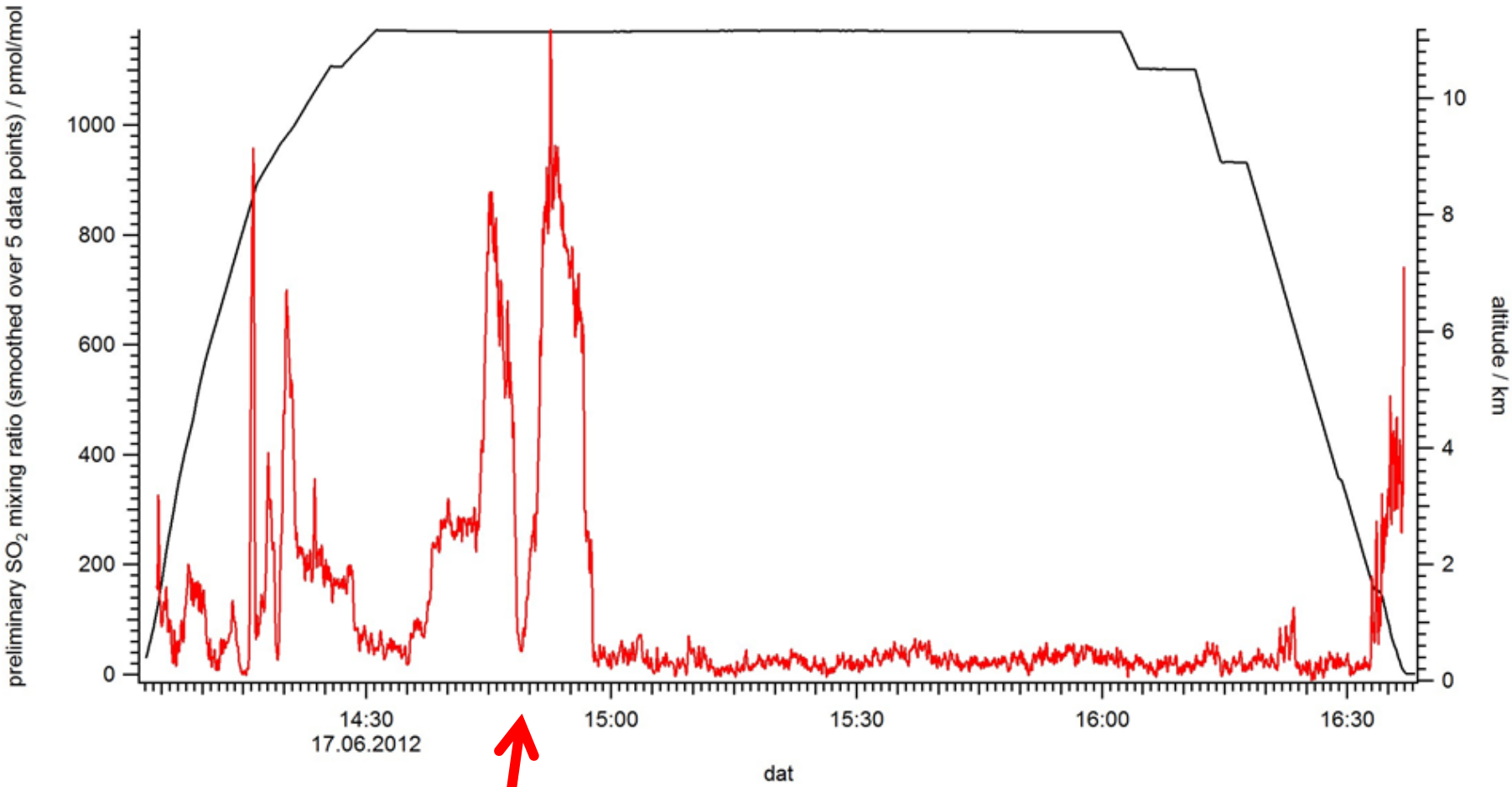


NO ~1 ppbv during >1 h at 11 km



Strong vertical uplift of pollution close to convection and UT/LS exchange

F120617a,
SO_2 timeseries, CI-ITMS



Strong vertical uplift of pollution close to convection and UT/LS exchange