AQRP 18-010
A synthesis study of the role of mesoscale and synoptic-scale wind on the concentrations of ozone and its precursors in Houston

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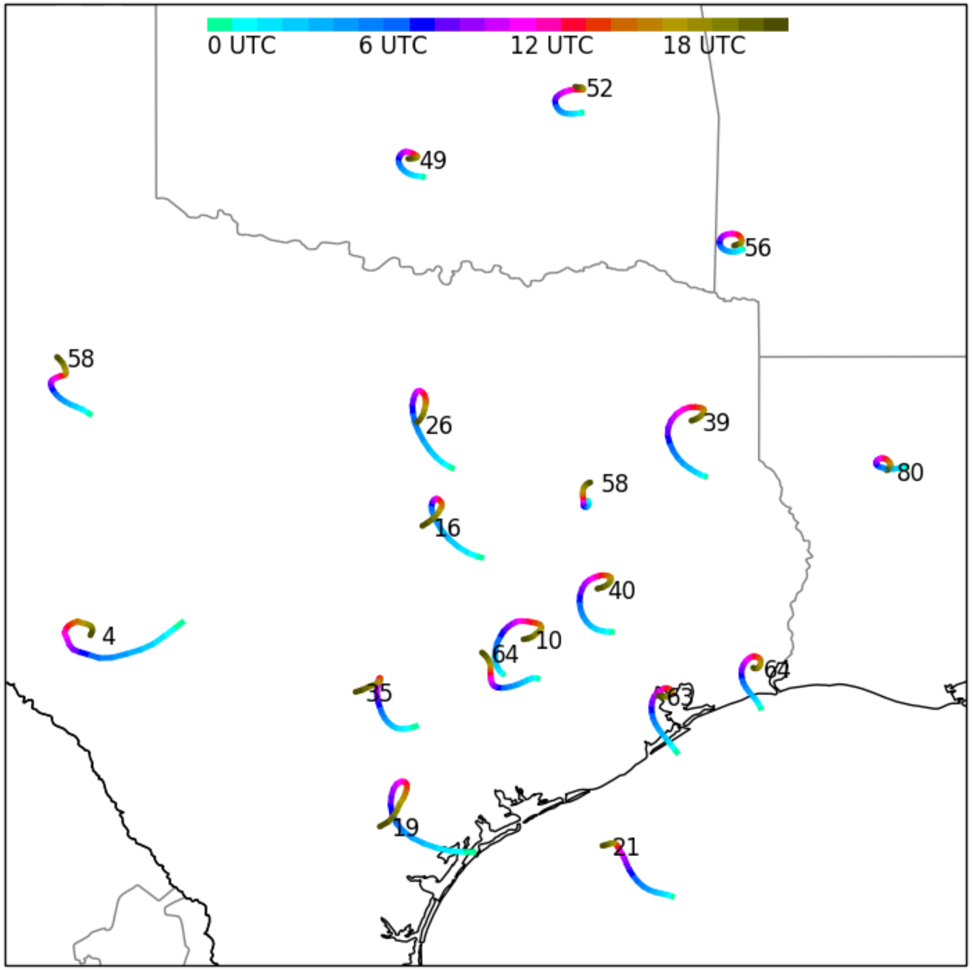


Composite analysis of mean air parcel trajectories under warm-season light wind conditions at 500 m above ground level, based on TexAQS-II profiler observations. Colors (bar at top) correspond to time of day (subtract six hours for LST), while numbers indicate the number of observed days meeting the low wind criterion.

Research Objective

- Synthesize existing data, previous analyses, and photochemical model experiments to provide a comprehensive and reconciled description of how mesoscale and synoptic-scale winds affect dispersion and accumulation of air pollutants emitted in the Houston area and from other regions, and how they contribute to high ozone events.

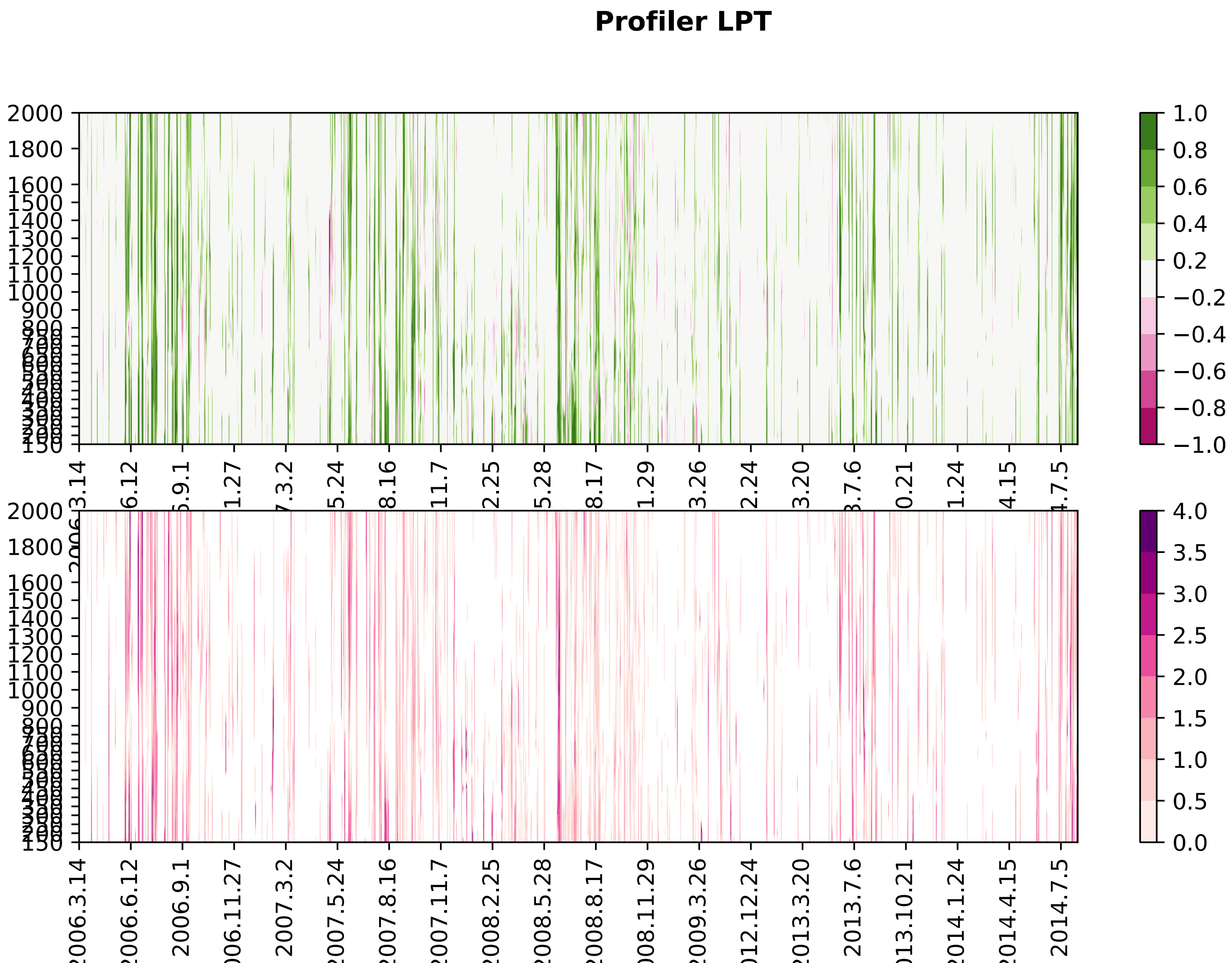
Tasks

- Task 1: Synthesis of mesoscale wind structures in synoptic-scale context
- Task 2: Development source and age resolved CMAQ model for ozone simulations
- Task 3: Analysis of interaction of mesoscale winds and ozone formation during key episodes

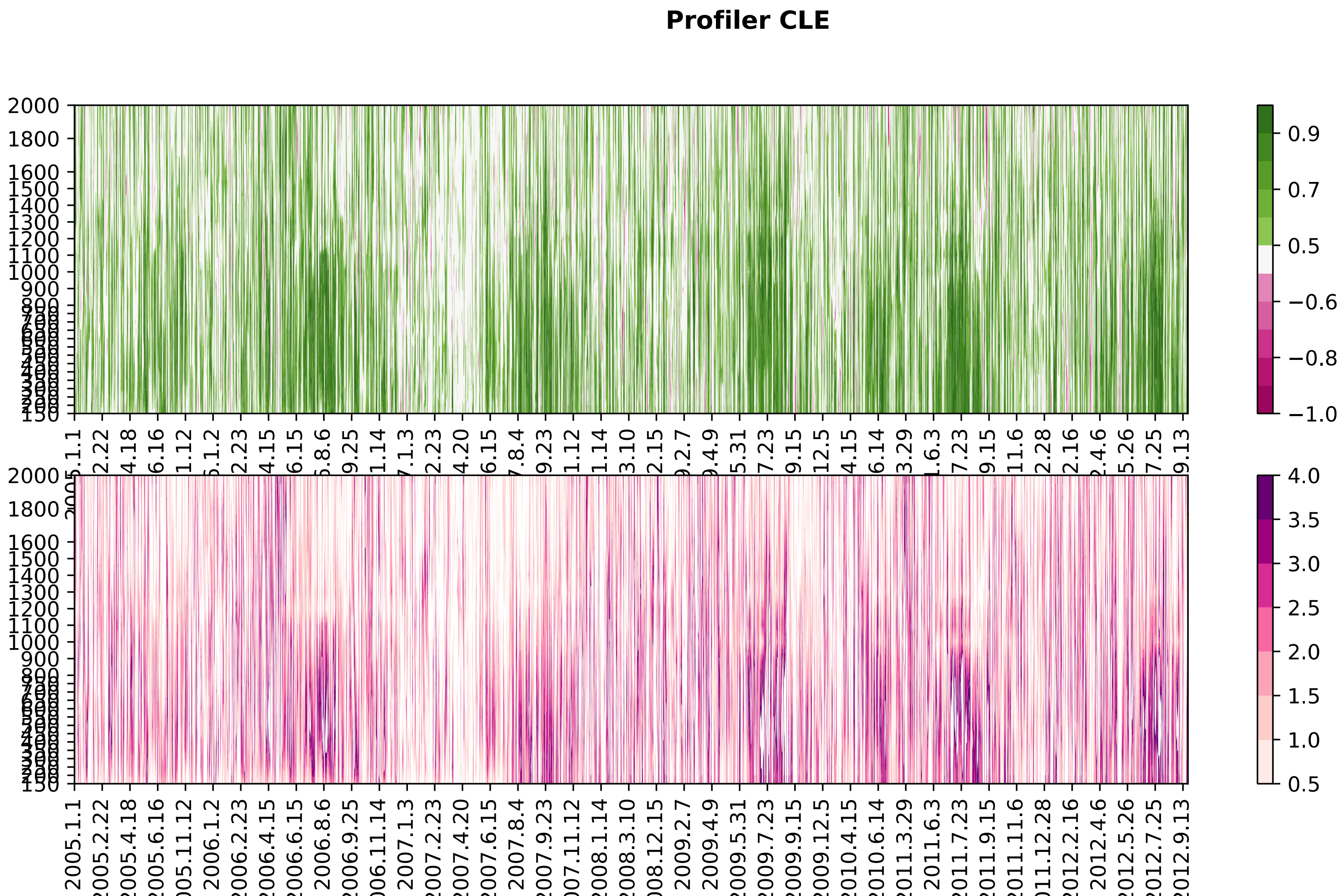
Task 1 Background: What CAN Drive Diurnal Wind Variations?

- Daytime heating, nighttime cooling, but what does that have to do with winds?
  - Possibility 1: Uneven heating (land vs. sea, etc.)
    - Result: Diurnally-varying horizontal pressure gradient
    - Winds respond
    - Ideal: light background pressure gradient/winds, strong heating
  - Possibility 2: Mixing and shear
    - Daytime heating mixes and slows winds in lowest 1-2 km
    - At night, mixing shuts off, winds respond to pressure at their own altitude
    - Ideal: strong background pressure gradient/winds, especially near ground

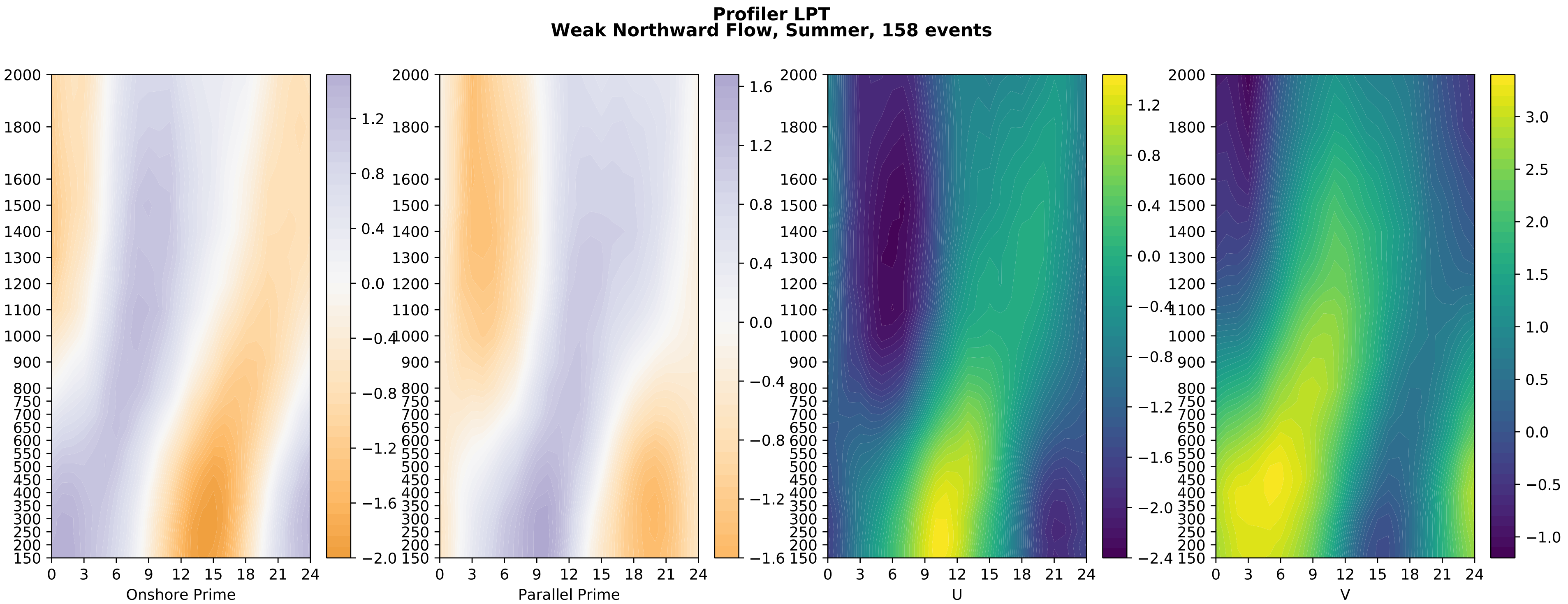
La Porte Diurnal Shape/Strength



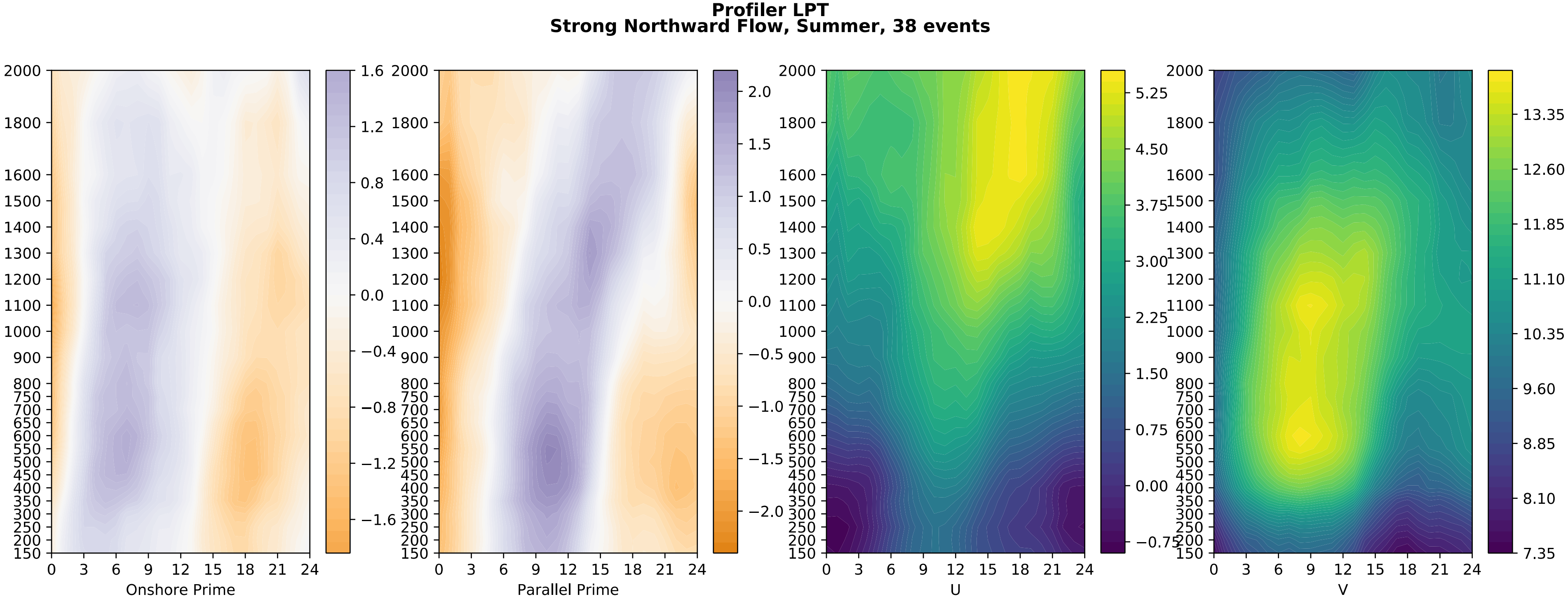
Cleburne Diurnal Shape/Strength



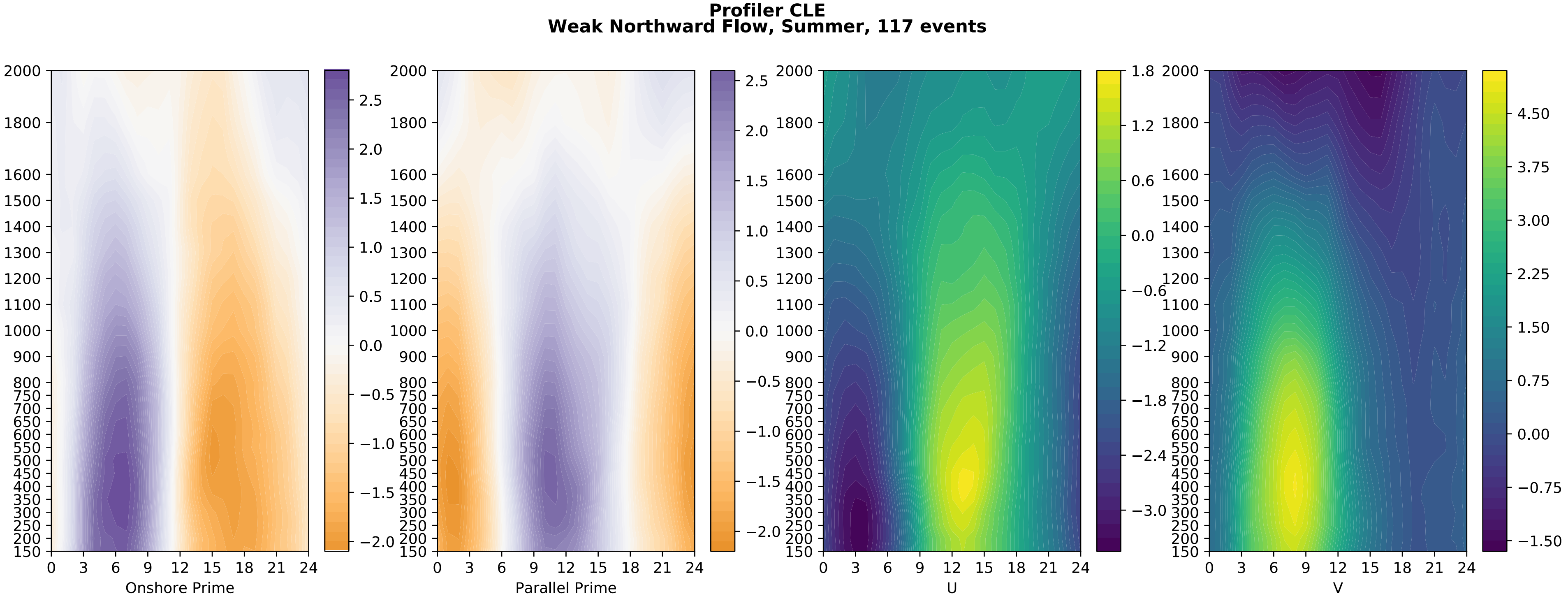
La Porte, Weak Southerly, AMJJAS



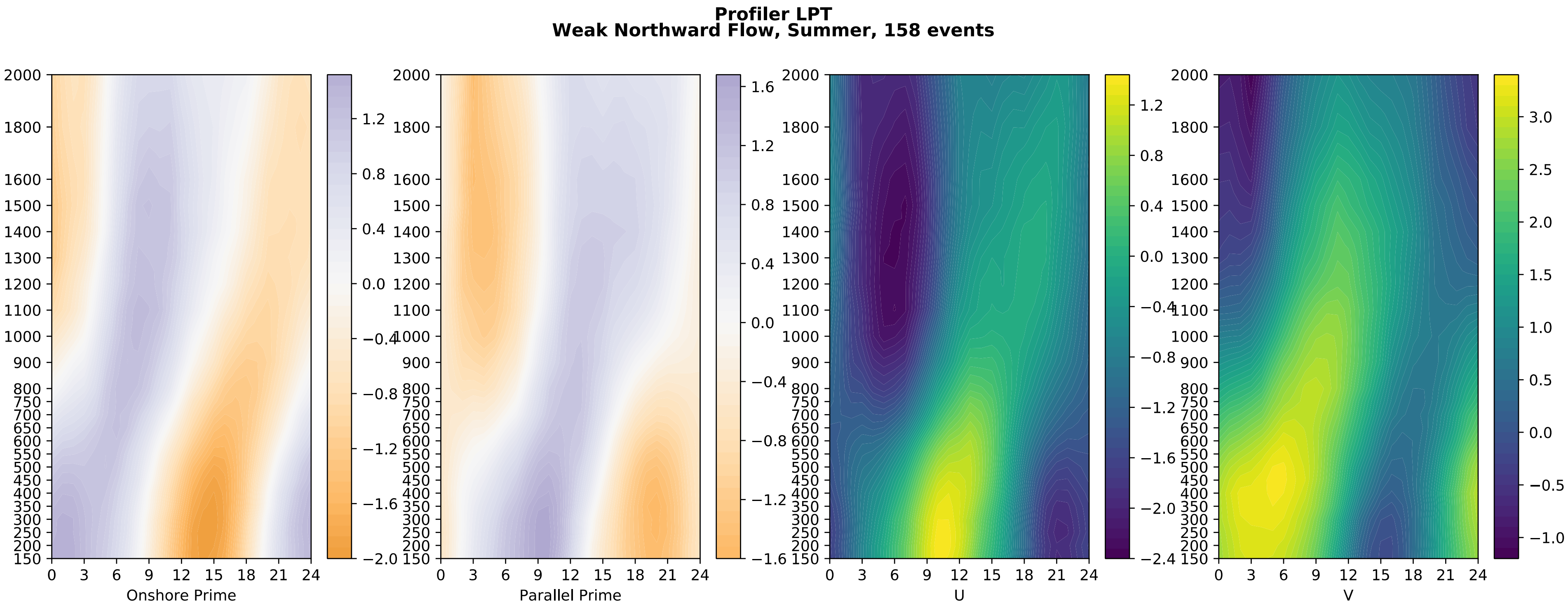
La Porte, Strong Southerly



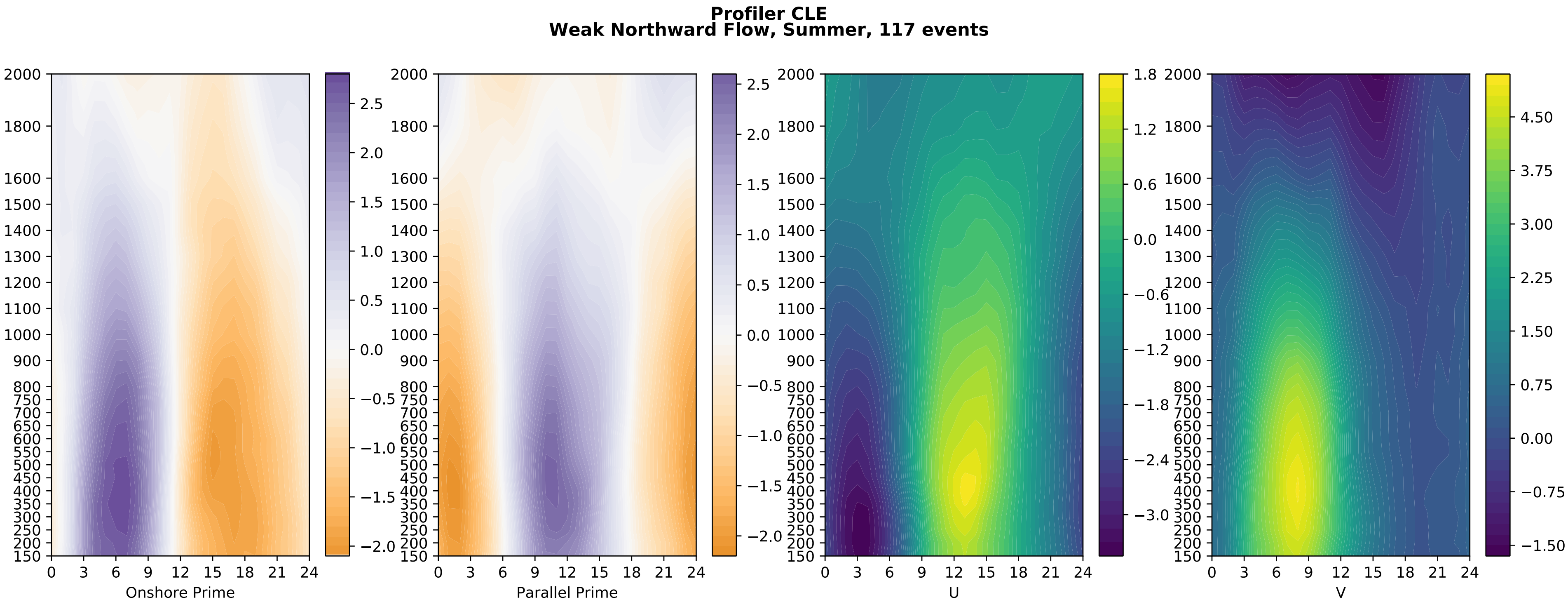
Cleburne, Weak Southerly



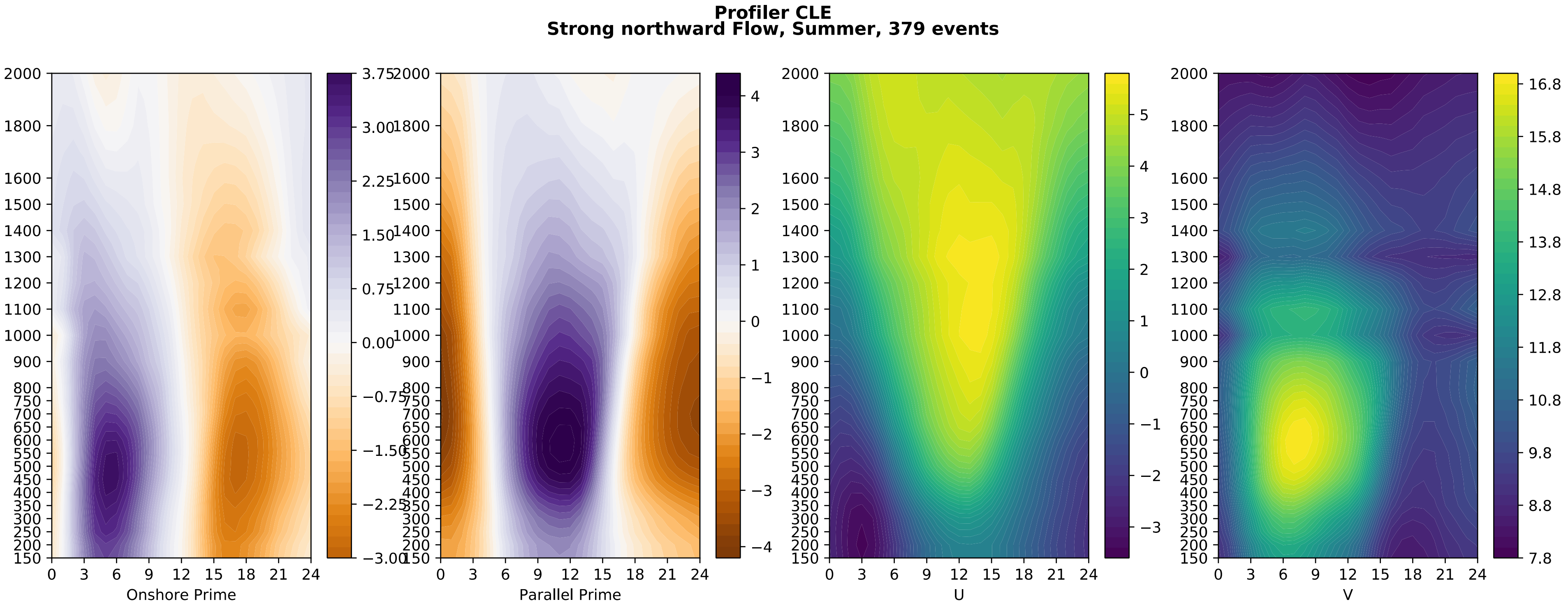
La Porte, Weak Southerly, AMJJAS



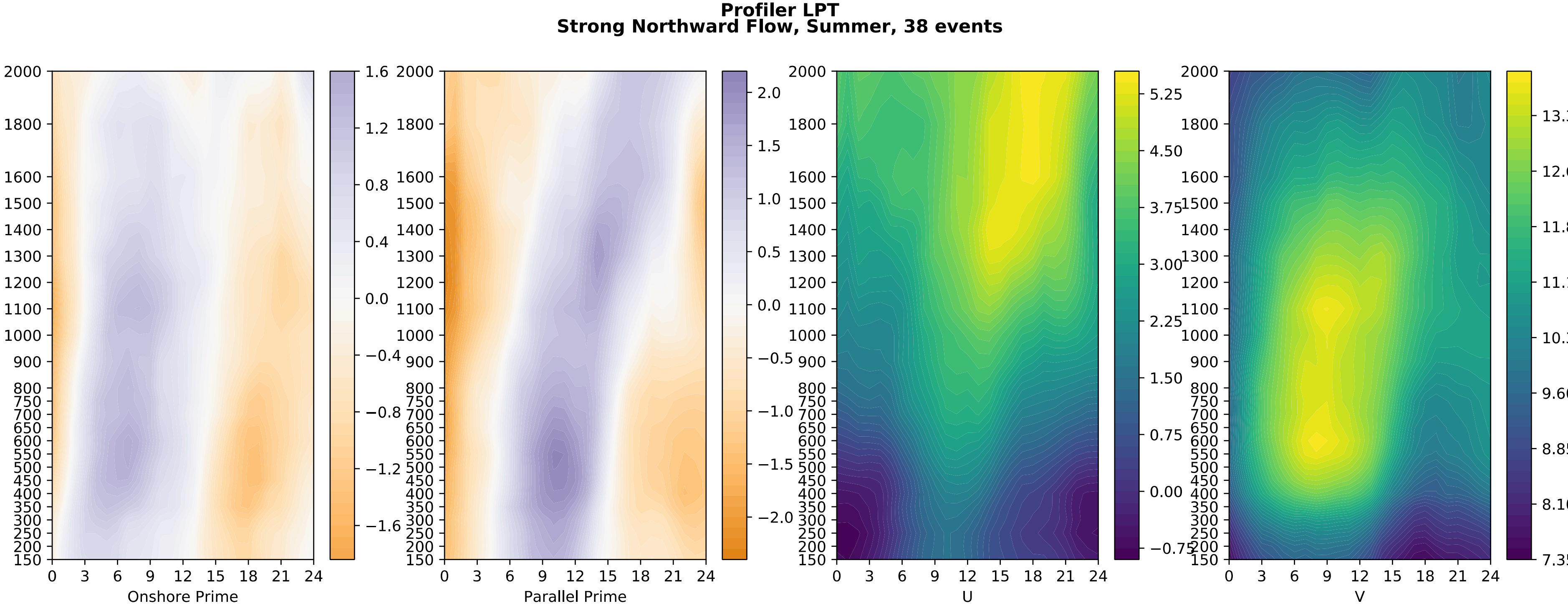
Cleburne, Weak Southerly



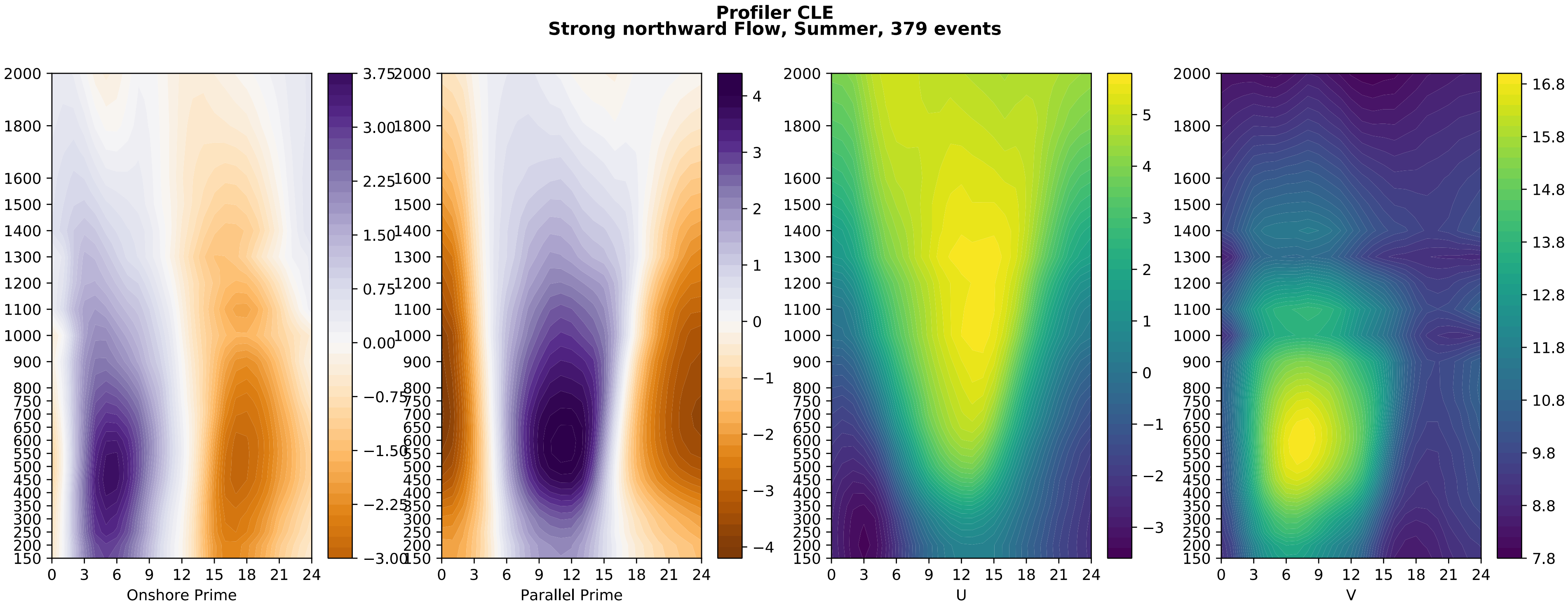
Cleburne, Strong Southerly

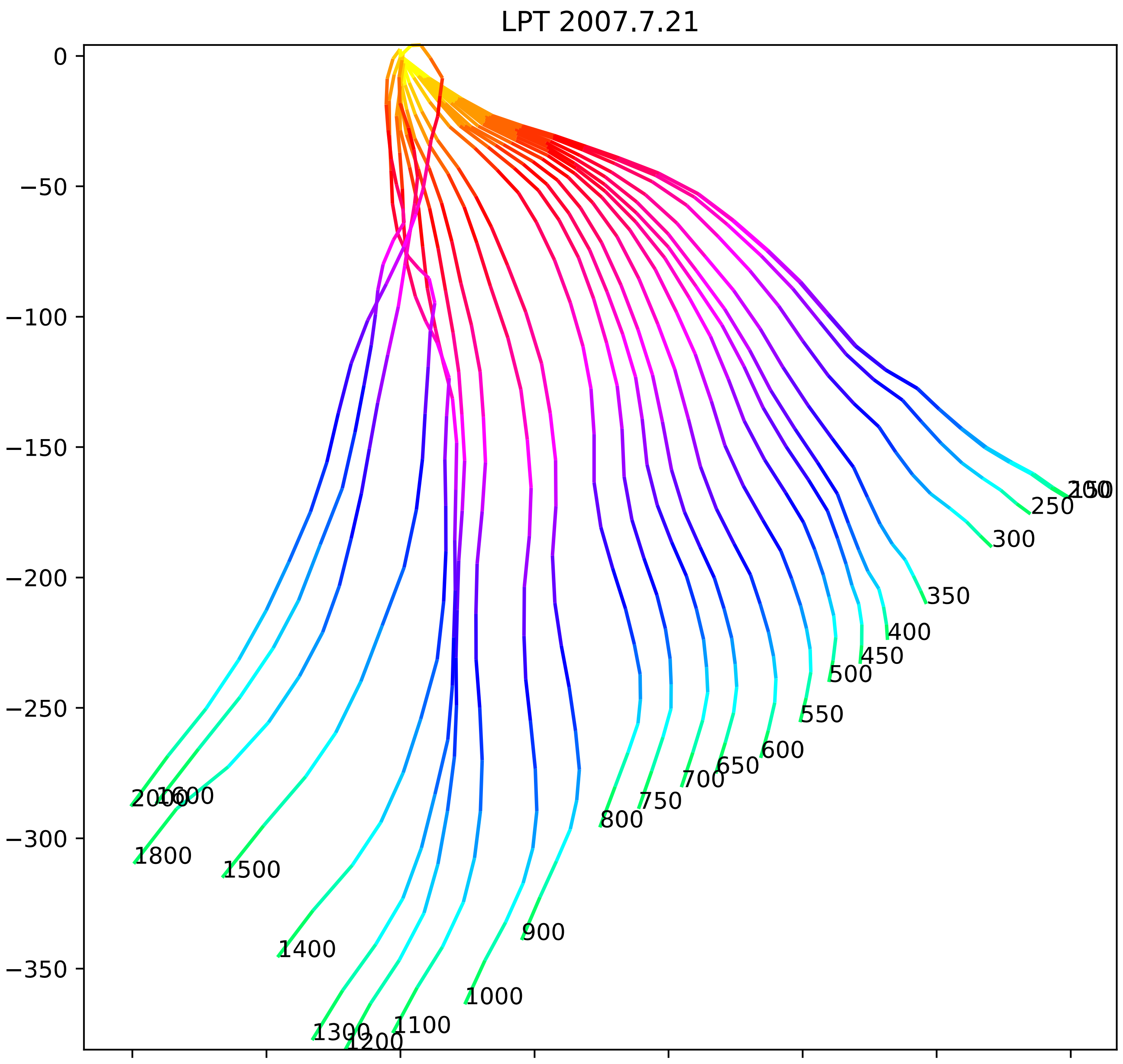


La Porte, Strong Southerly

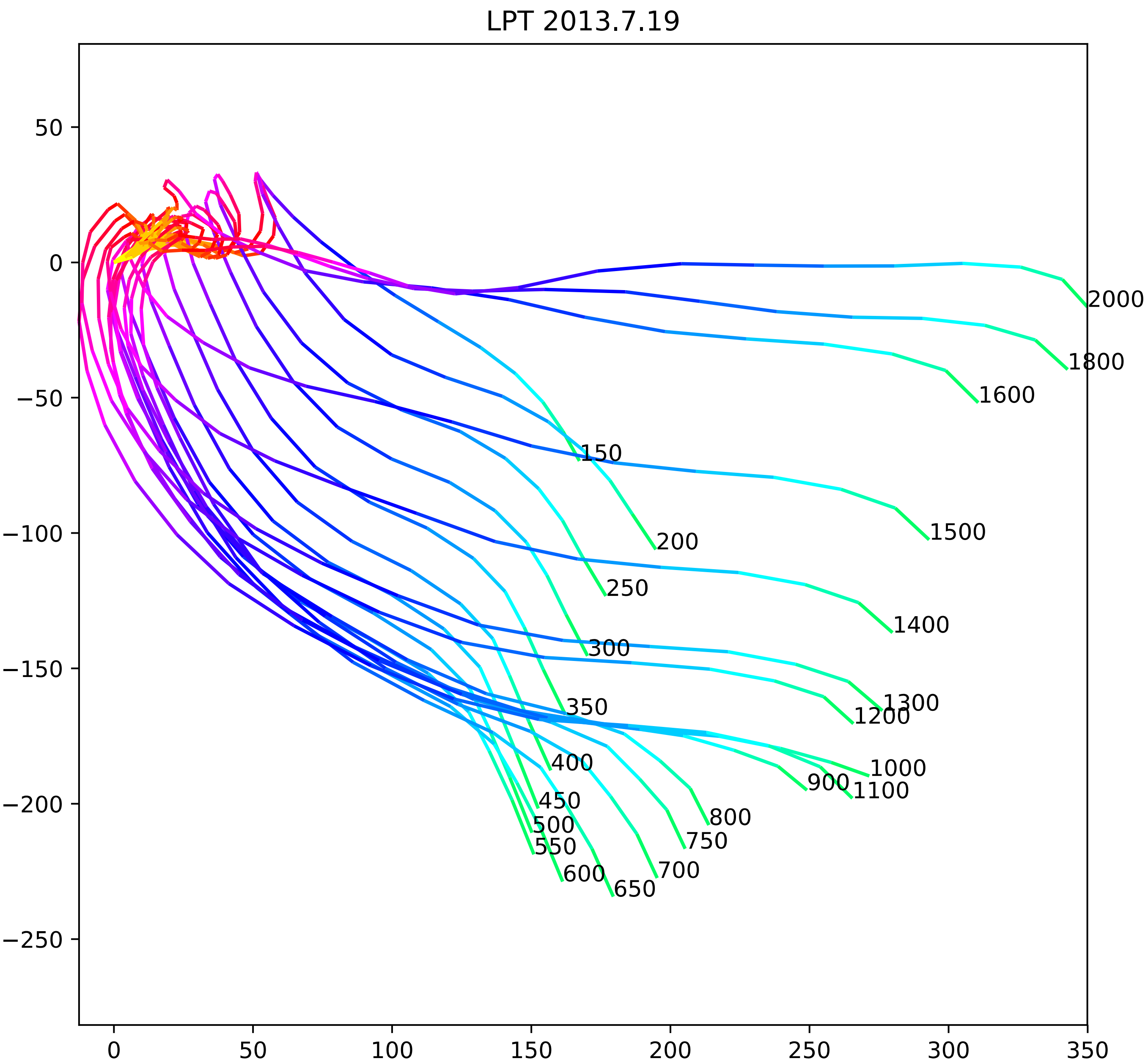


Cleburne, Strong Southerly





LPT 2007.7.21
0
−50
−100
−150
−200
−250
−300
−350
−100
−50
0
50
100
150
200
250
150
200
250
300
350
400
450
500
550
600
650
700
750
800
900
1000
1100
1200
1300
1400
1500
1600
1800
2000


LPT 2013.7.19
50
0
−50
−100
−150
−200
−250
0
50
100
150
200
250
300
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2000
1800
1600
150
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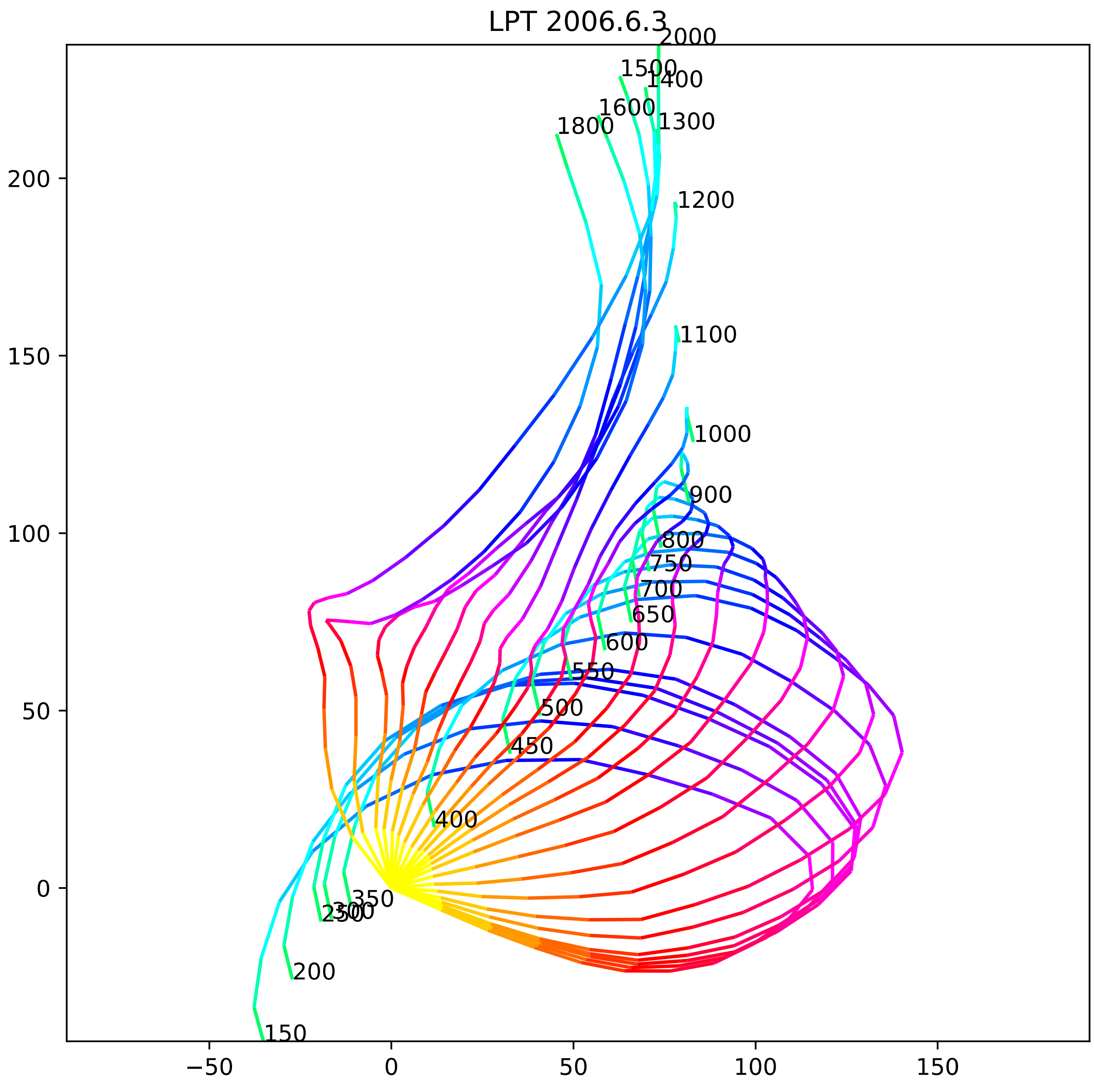
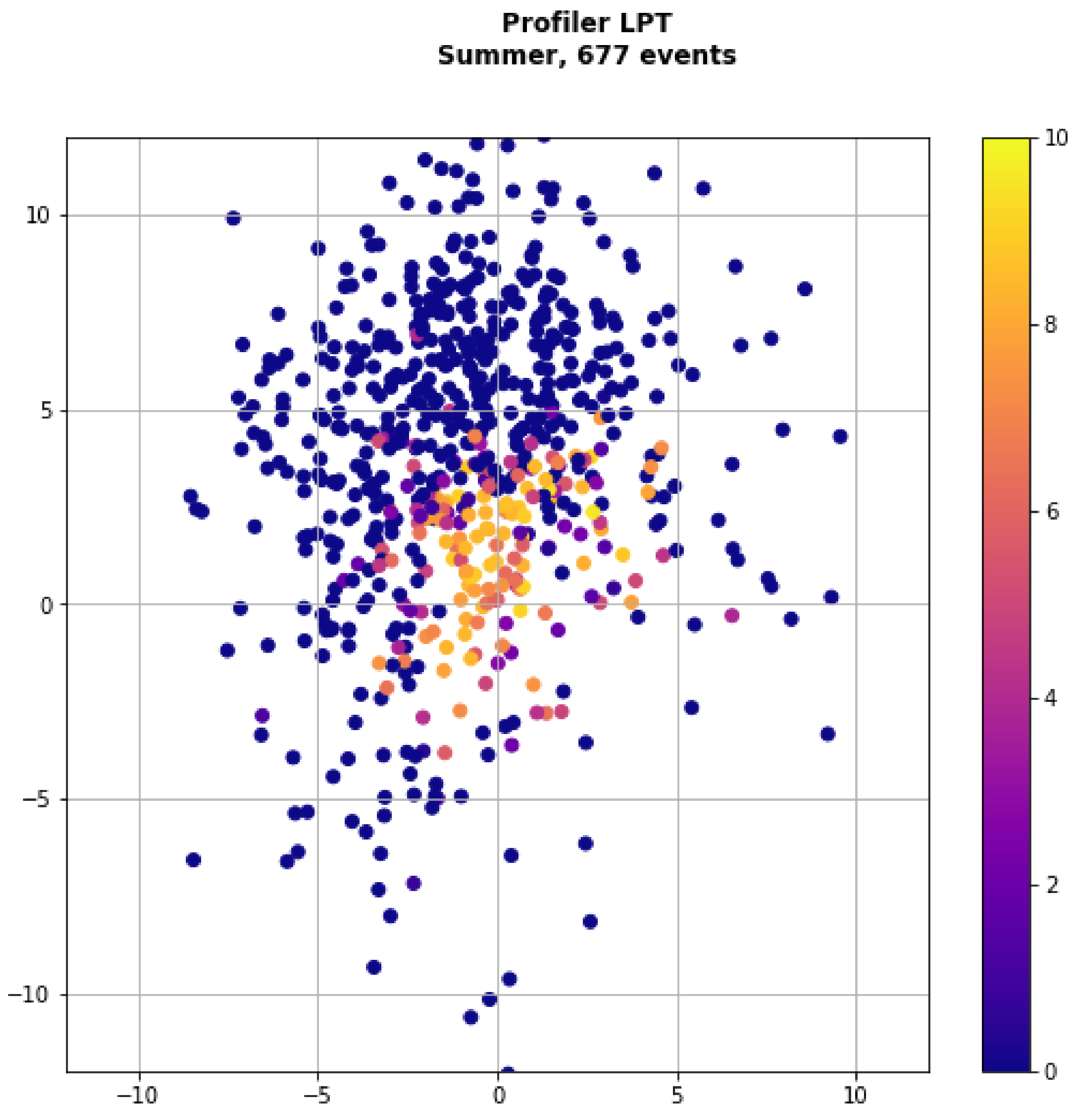
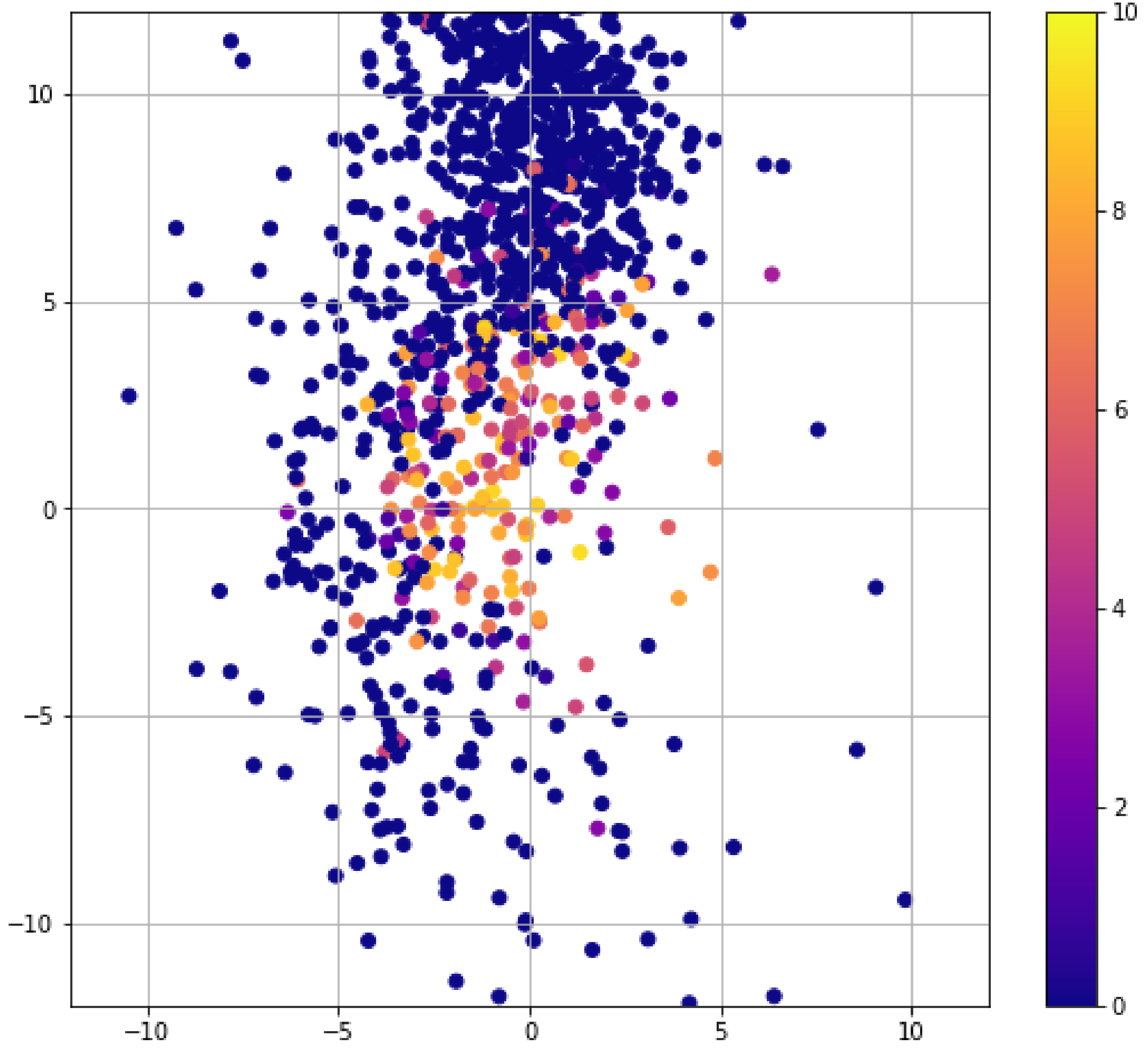
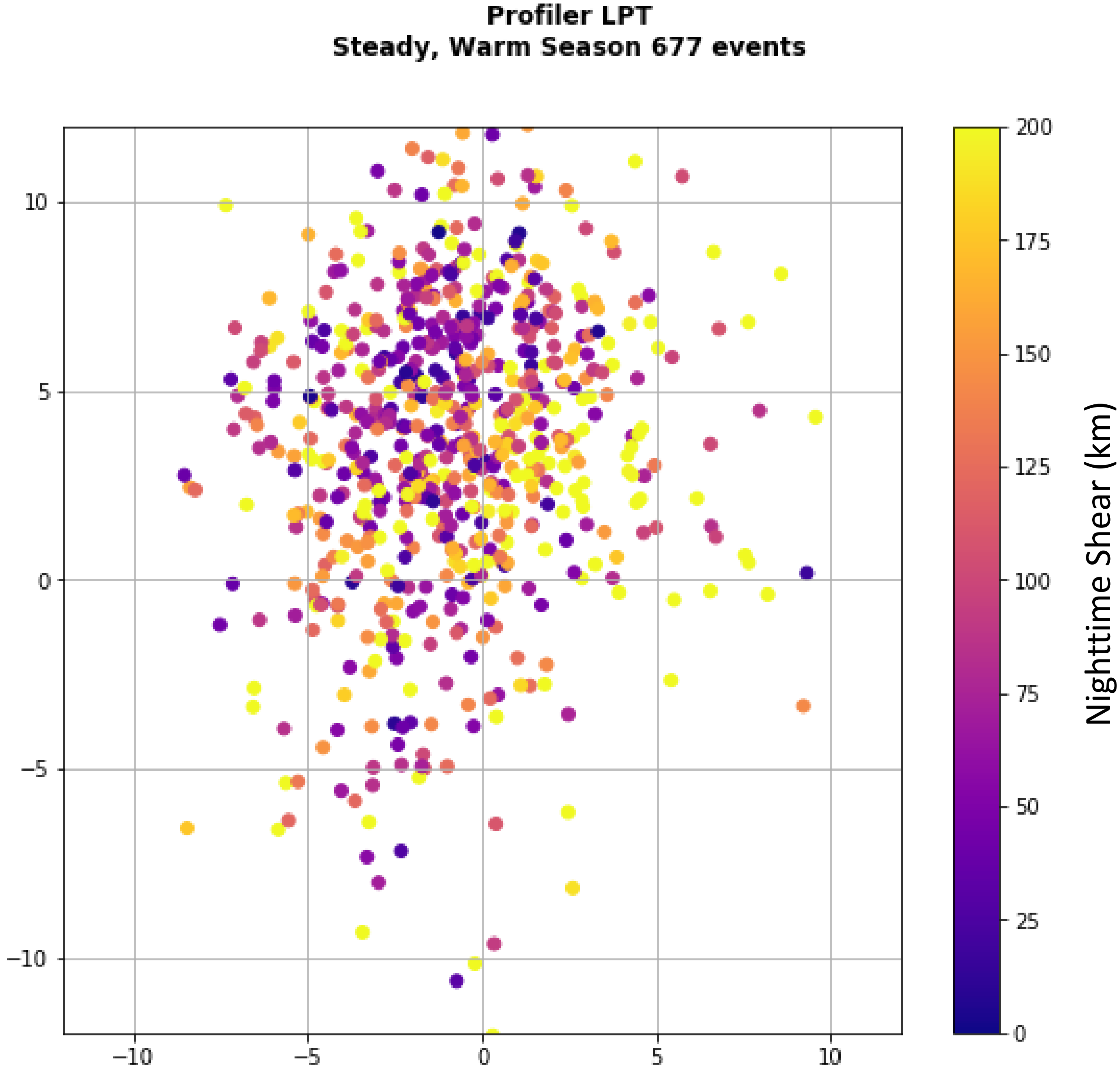
750
550
700
600
650


LPT 2006.6.3
2000
1500
1400
1600
1300
1800
1200
1100
1000
900
800
750
700
650
600
550
500
450
400
350
300
250
200
150
200
150
100
50
0
−50
0
50
100
150


Profiler LPT
Summer, 677 events
10
5
0
−5
−10
−10
−5
0
5
10
10
8
6
4
2
0

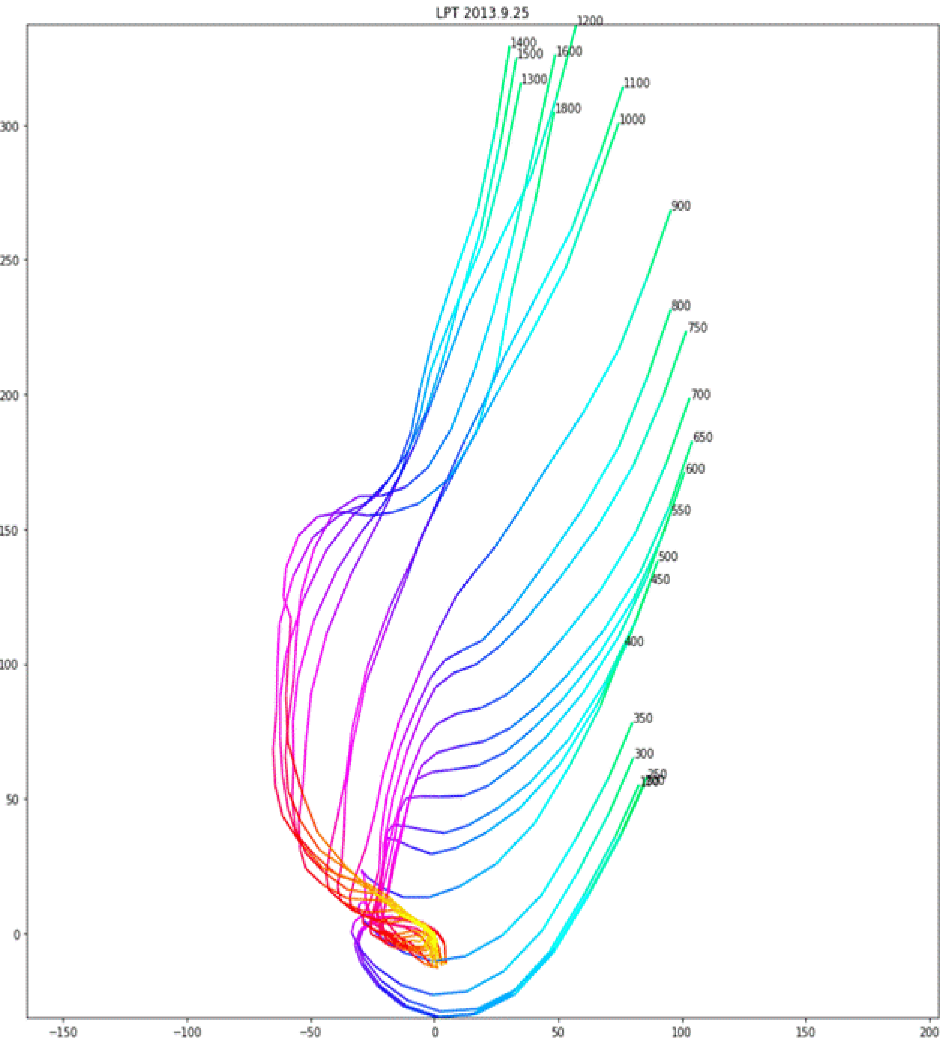
Profiler CLE
Steady, Warm Season 1232 events

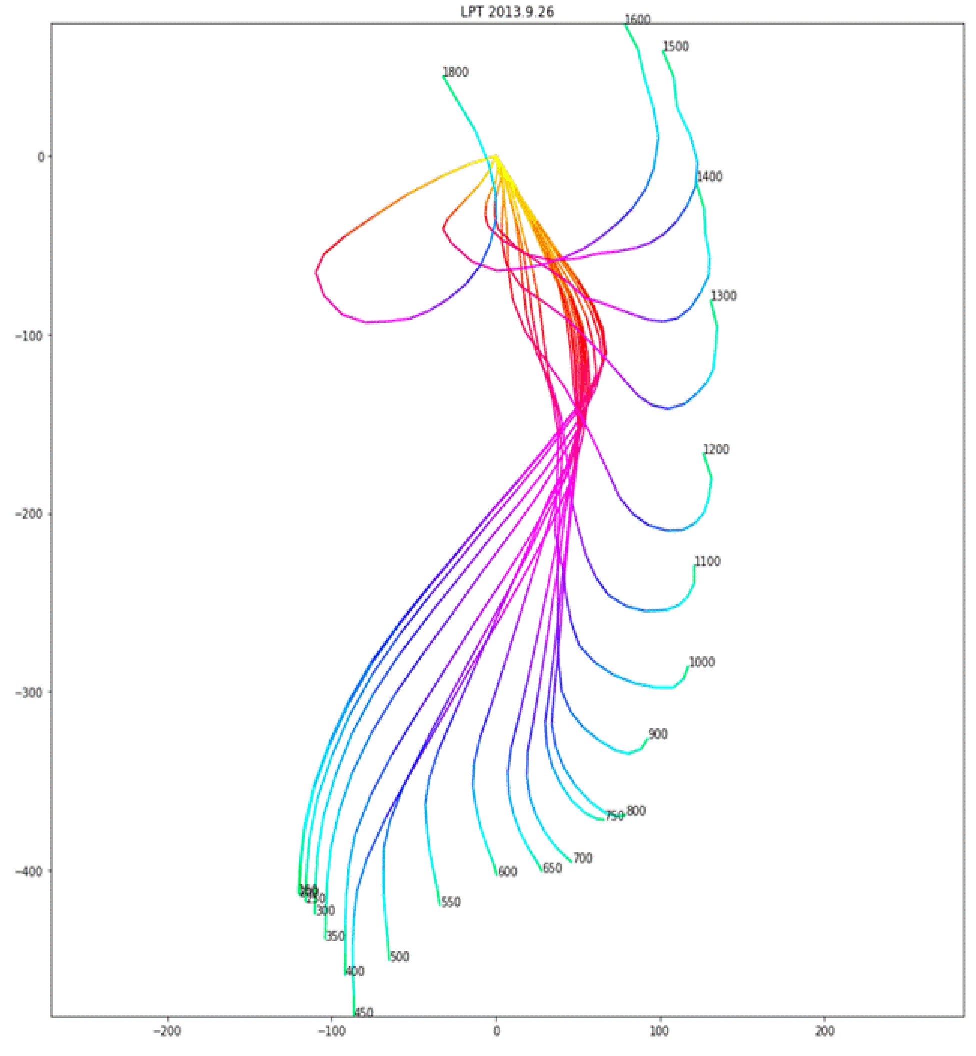




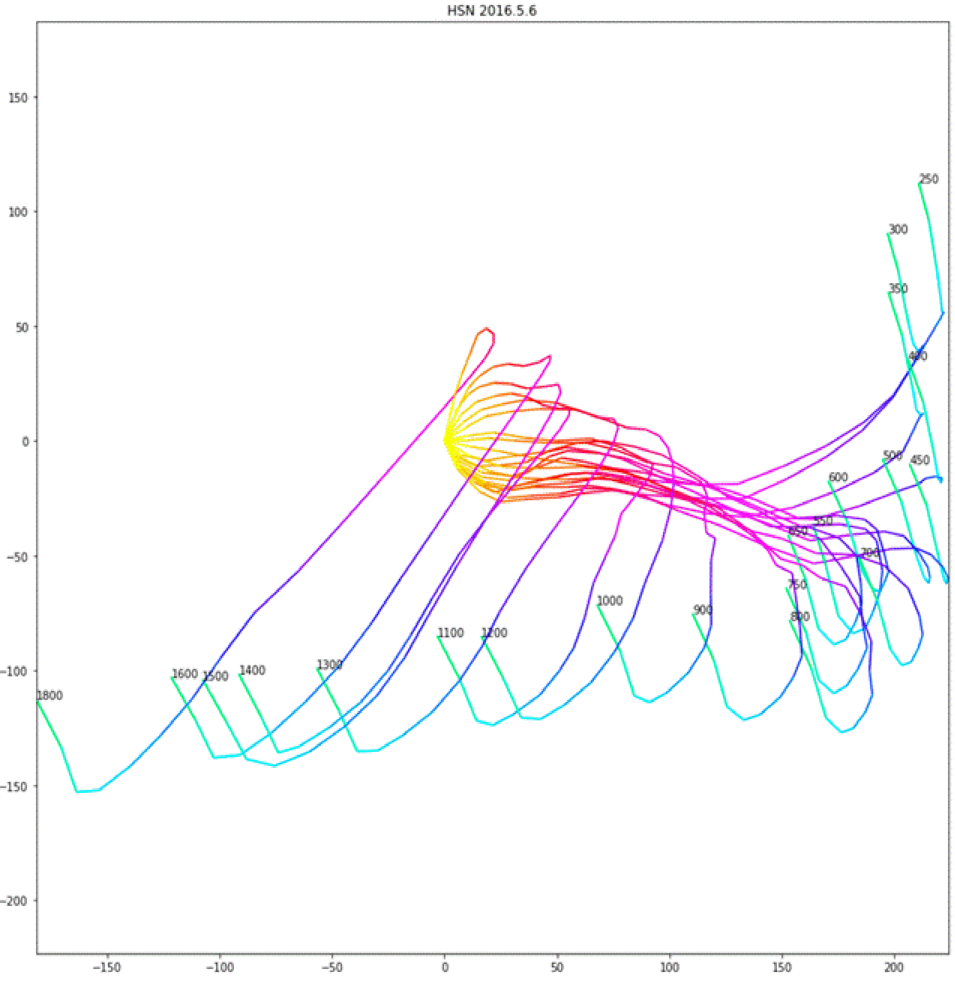
Profiler LPT
Steady, Warm Season 677 events
10
5
0
−5
−10
−10
−5
0
5
10
200
175
150
125
100
75
50
25
0
Nighttime Shear (km)

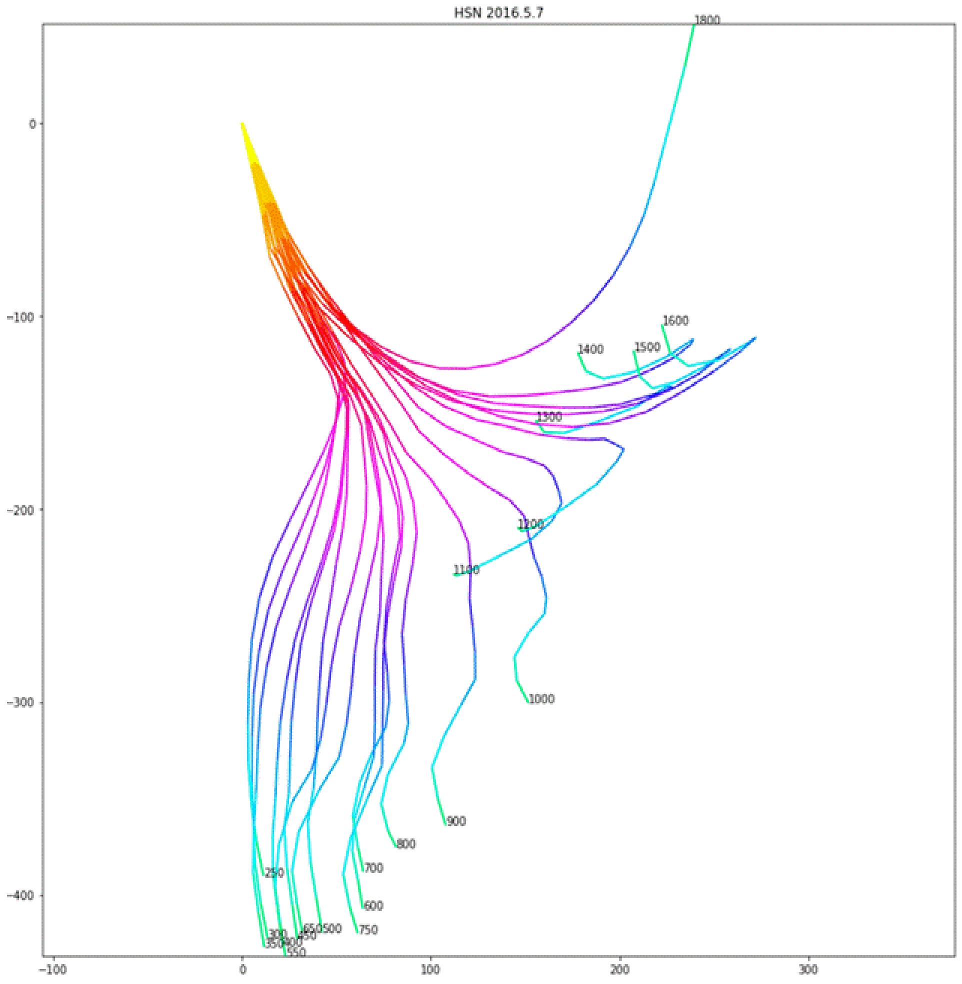
September 2013 case: 124 ppb



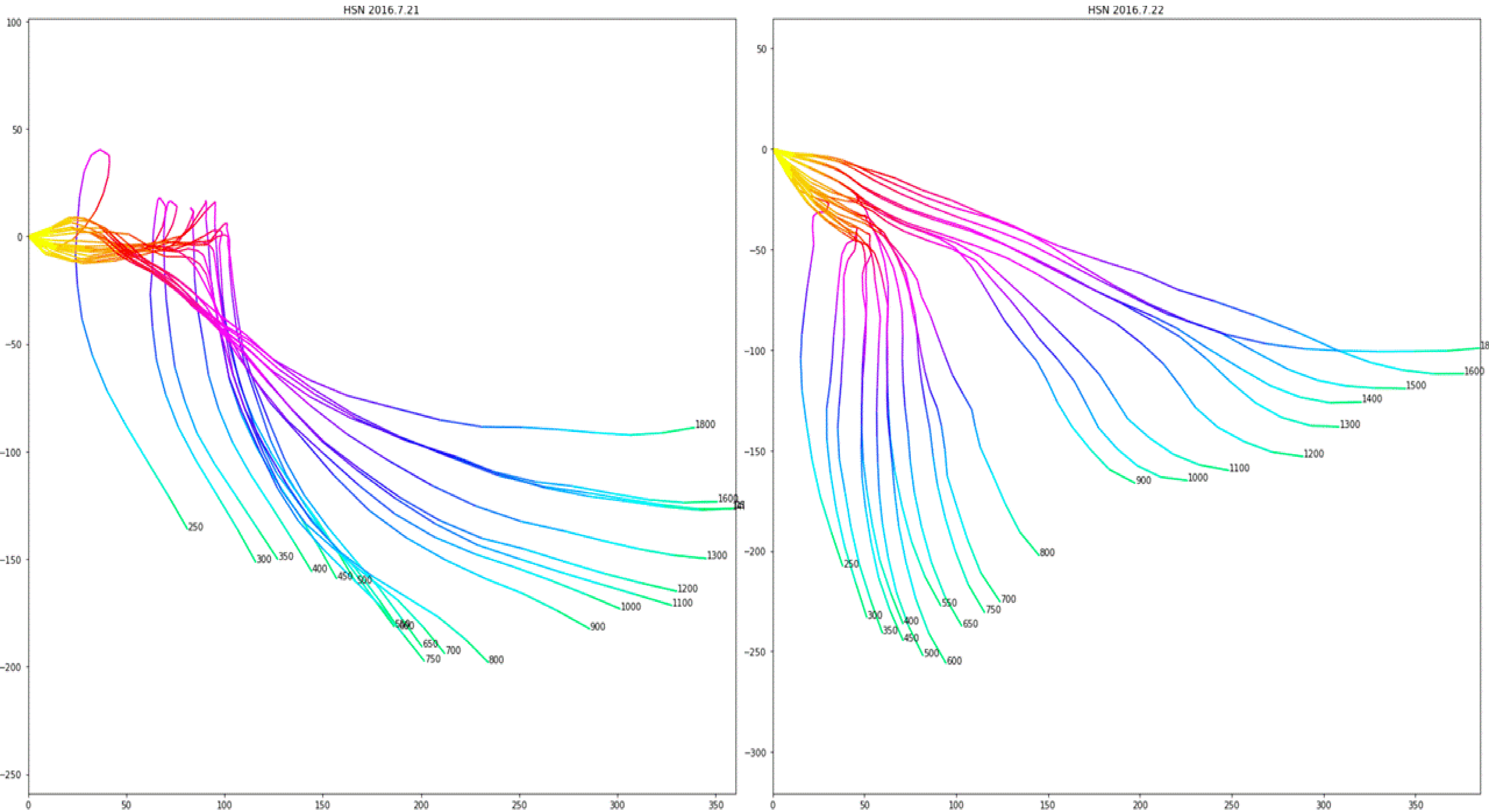


May 2016 case: 89 ppb





July 2016 case: 85 ppb

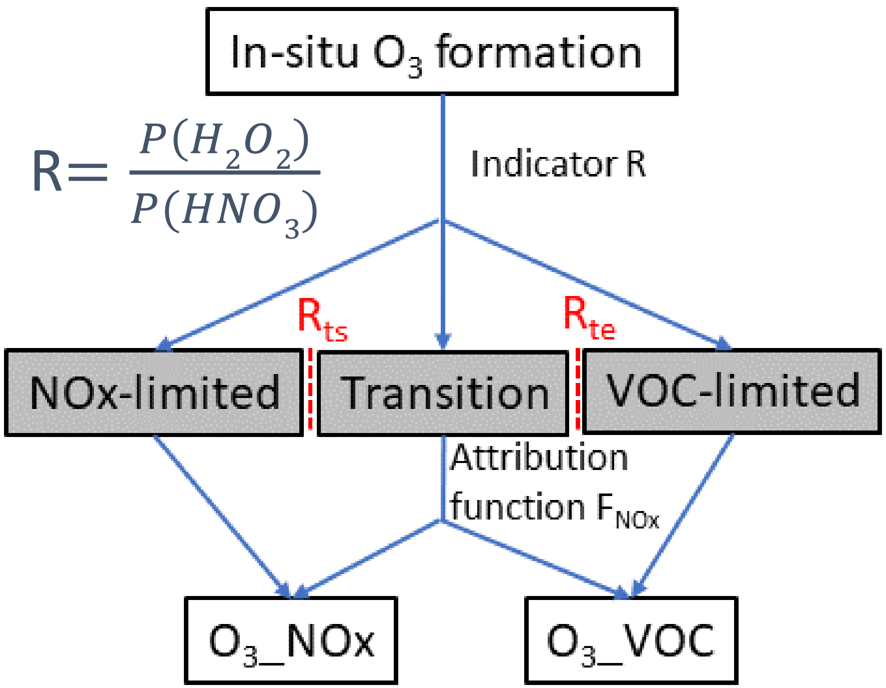


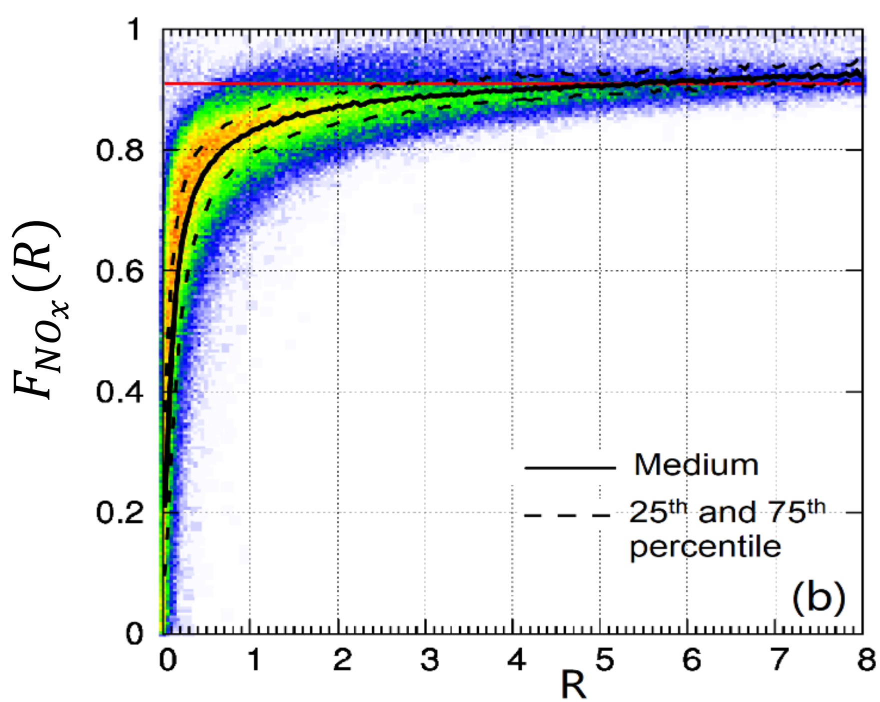
Task 2: Development source and age resolved CMAQ model for ozone simulations

Task 2: Modeling atmospheric age distribution of ozone in CMAQ

Step 1: Attributing O_3 to NOx and VOC based on sensitivity regime

$$F_{NO_x}(R) = \frac{\delta O_3^{NO_x}(R)}{\delta O_3^{VOC}(R) + \delta O_3^{NO_x}(R)}$$

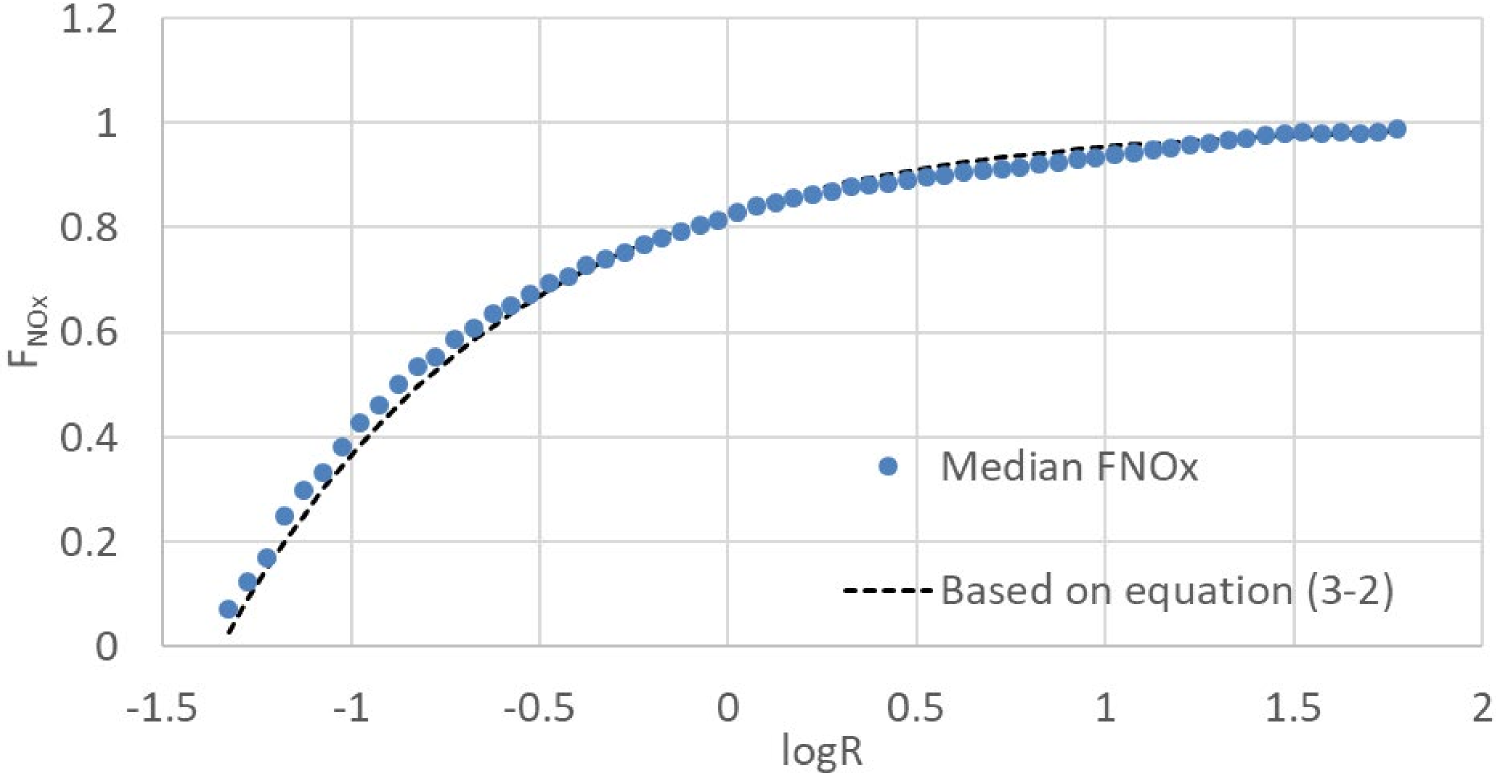




Wang et al., ES&T, 53(3), 1404-1412

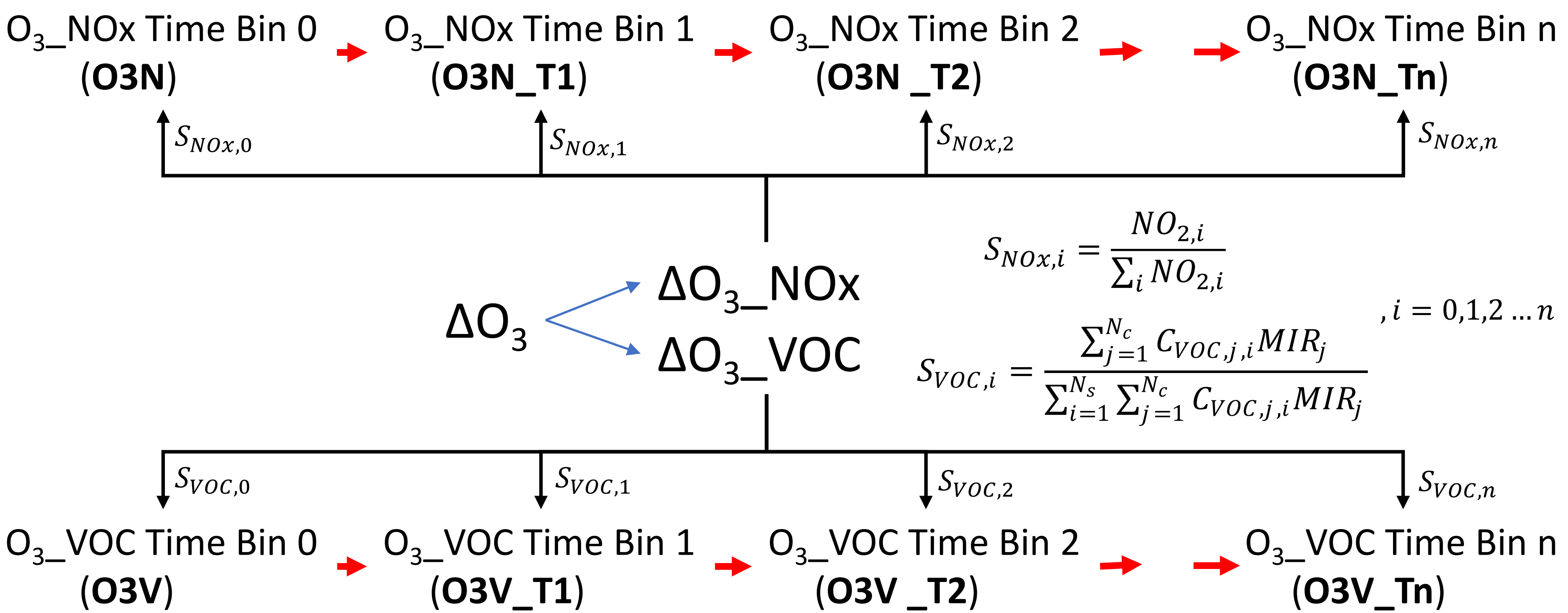
New Parameterization for F_{NOx}

$F_{NOx} = 1.0 - 0.1715exp(-1.309log_{10}R)$ (equation 3.2)



Modeling atmospheric age distribution of ozone

Step 2: Attributing O_3_NOx and O_3_VOC to different age groups based on the atmospheric age distribution of NOx and VOCs

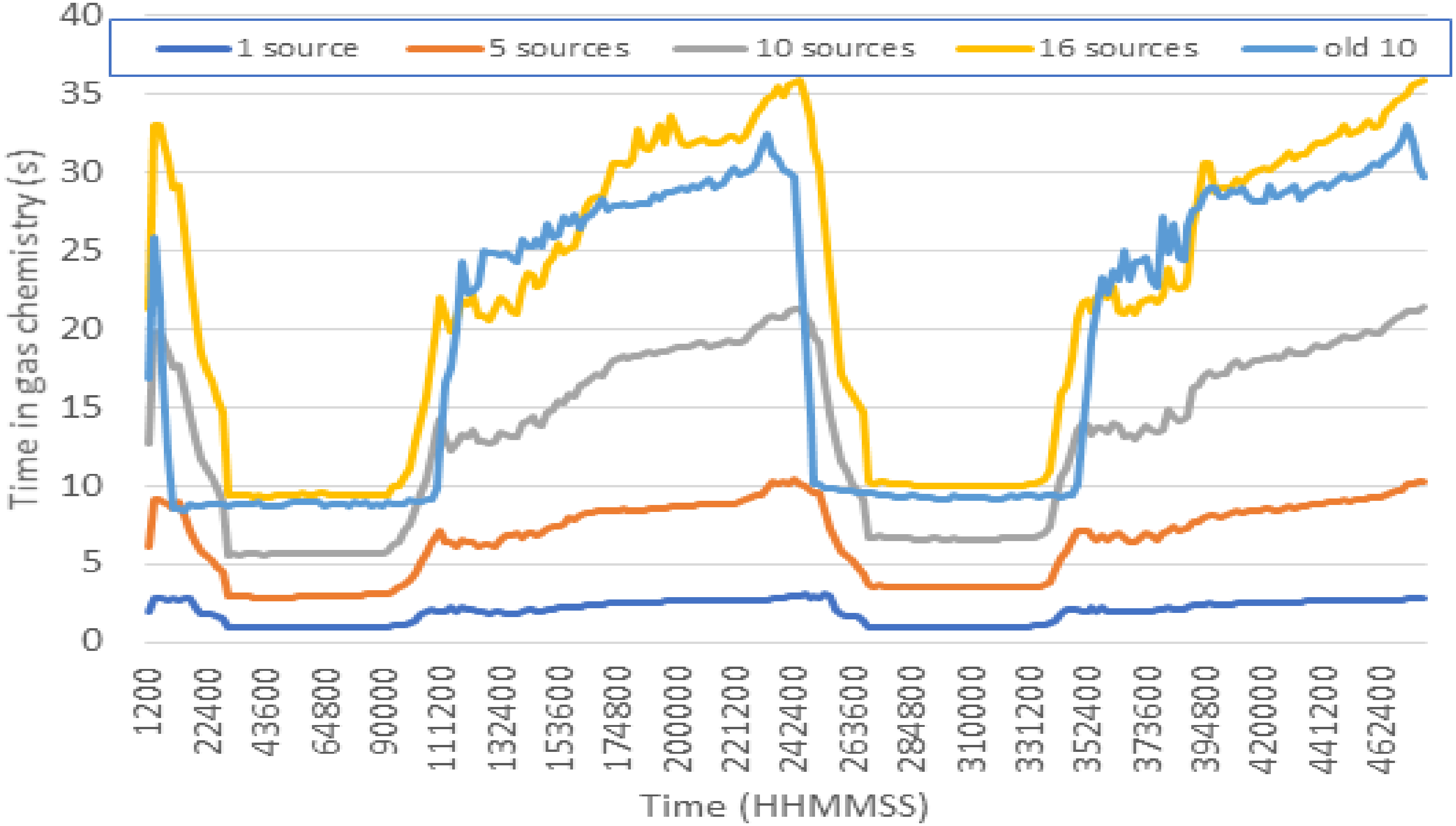


→ Advance in time bin, based on a predefined advancing frequency

→ Formation of O3_NOx and O3_VOC, at each model time step

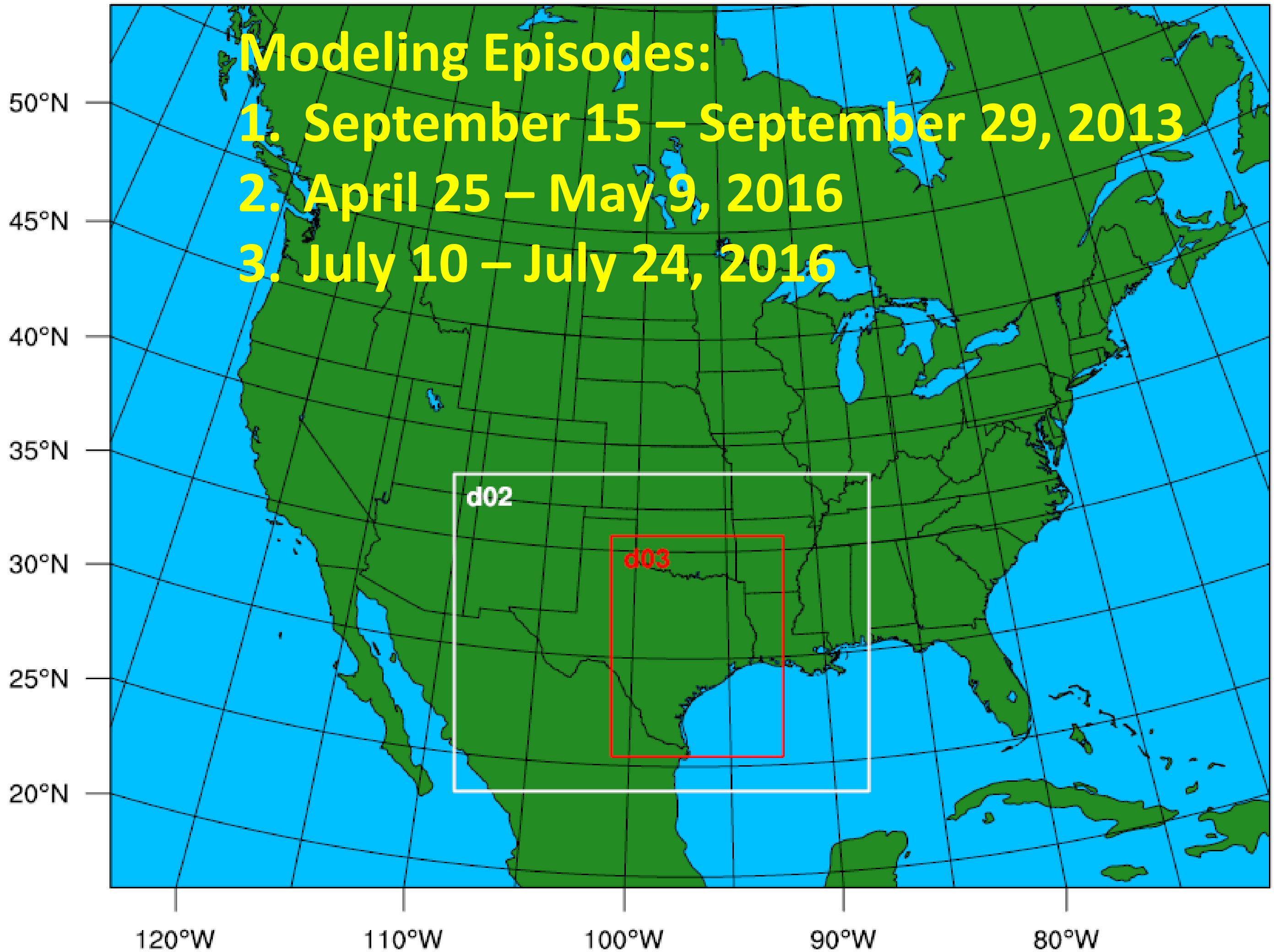
Computation efficiency improvement

Wall-clock time in gas phase chemistry during a two-day simulation with various number of sources to track

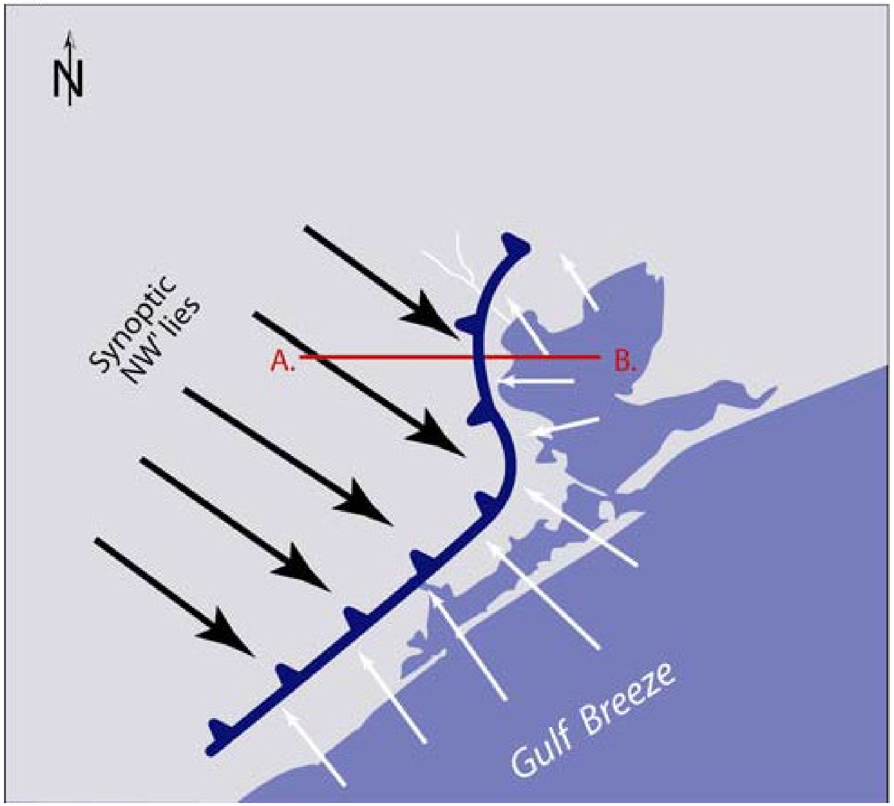


Task 3: Analysis of interaction of mesoscale winds and ozone formation during key episodes

WRF/CMAQ Model Domains

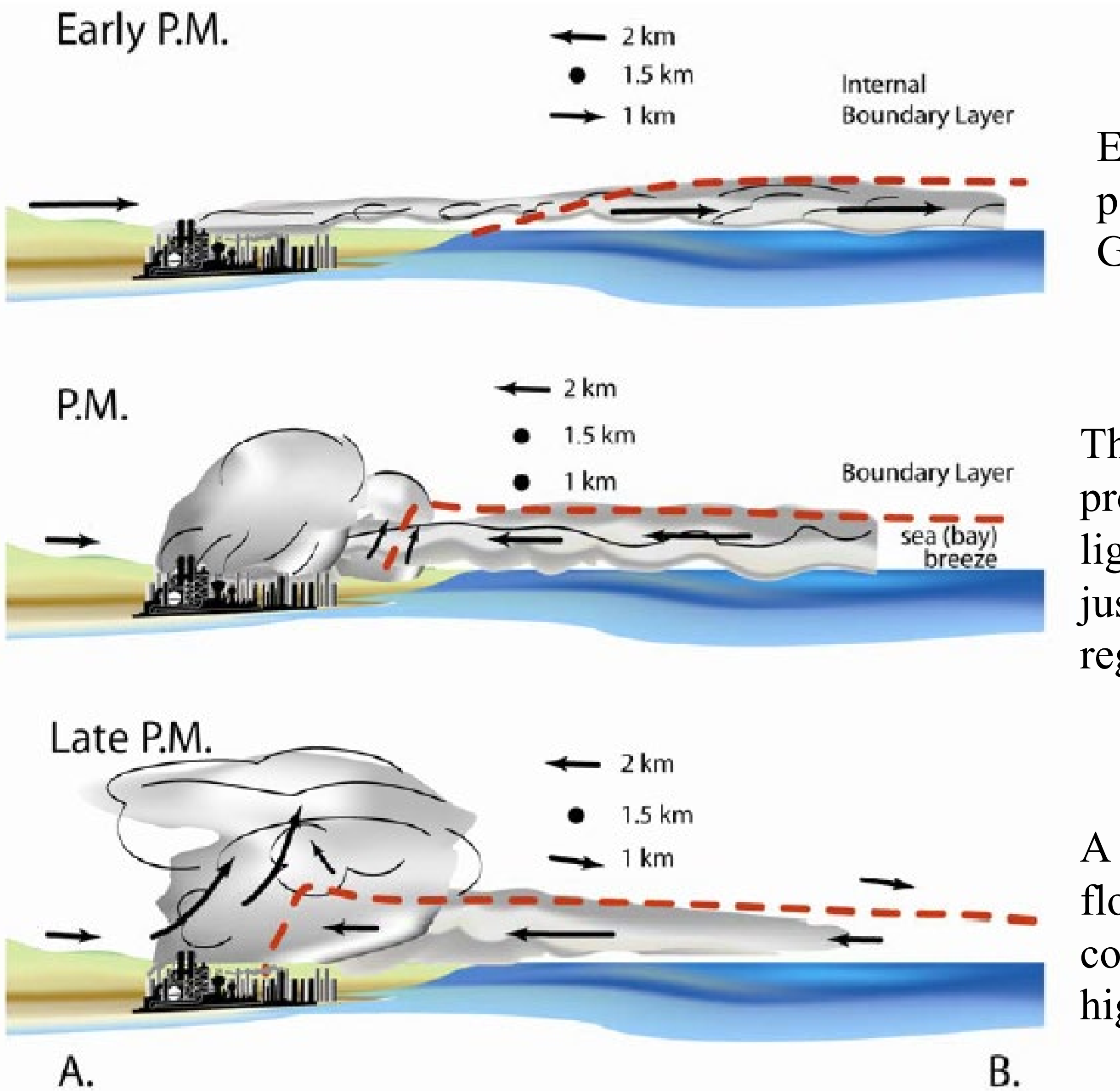


Synoptic NW’lies and the Gulf Breeze



Banta et al., 2005

Schematic vertical cross section along line AB



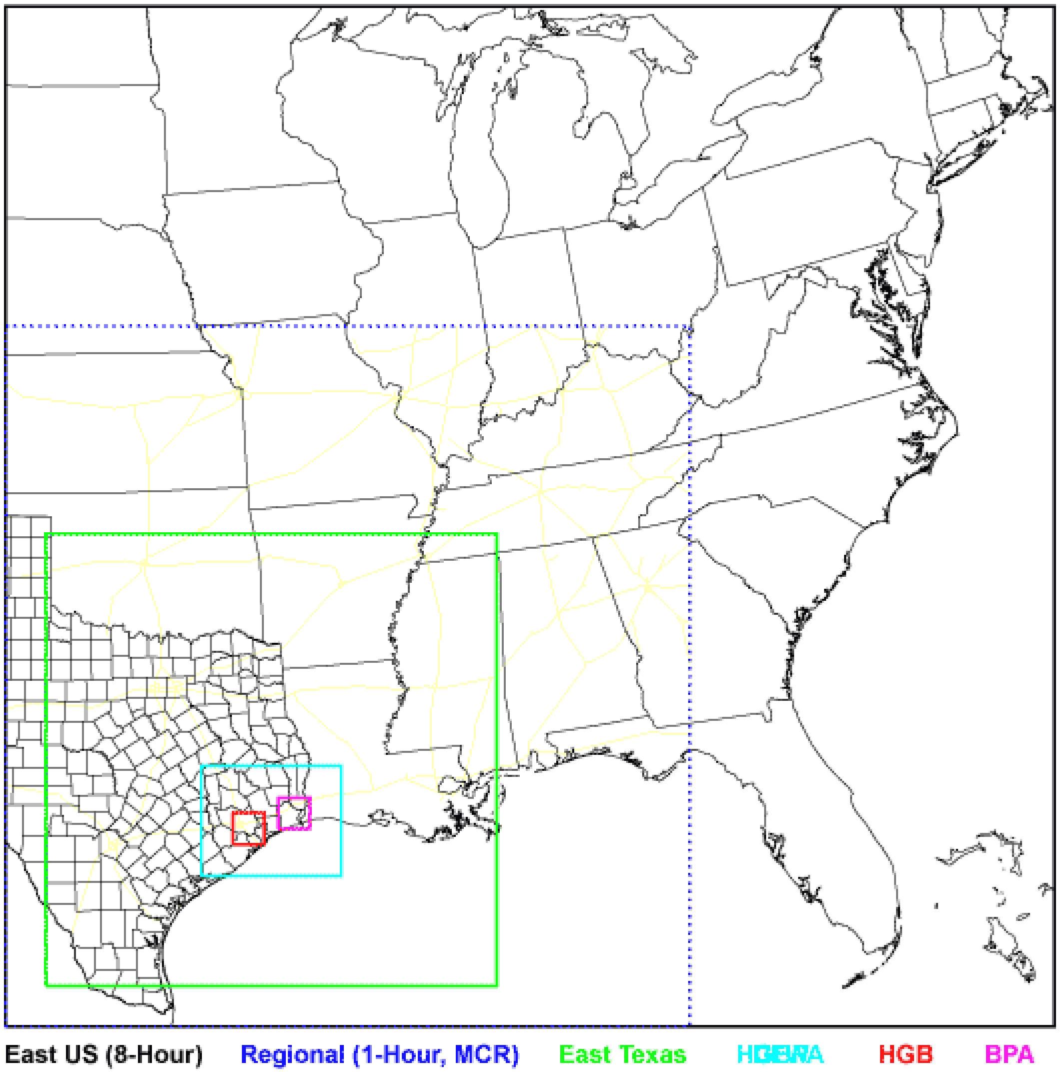
Early-day offshore flow taking pollutants outward over Galveston Bay

The incipient Bay breeze producing a convergence zone of light and variable surface winds just onshore over the source regions,

A more fully developed onshore flow producing stronger convergence, lofting pollutants high over the coastal zone.

Banta et al., 2005

Case 1: August 2000 (TexAQS 2000)



Episode: 8/15 – 9/6, 2000
Meteorology: MM5
Emissions: BEIS + NEI + Texas Specific Emissions

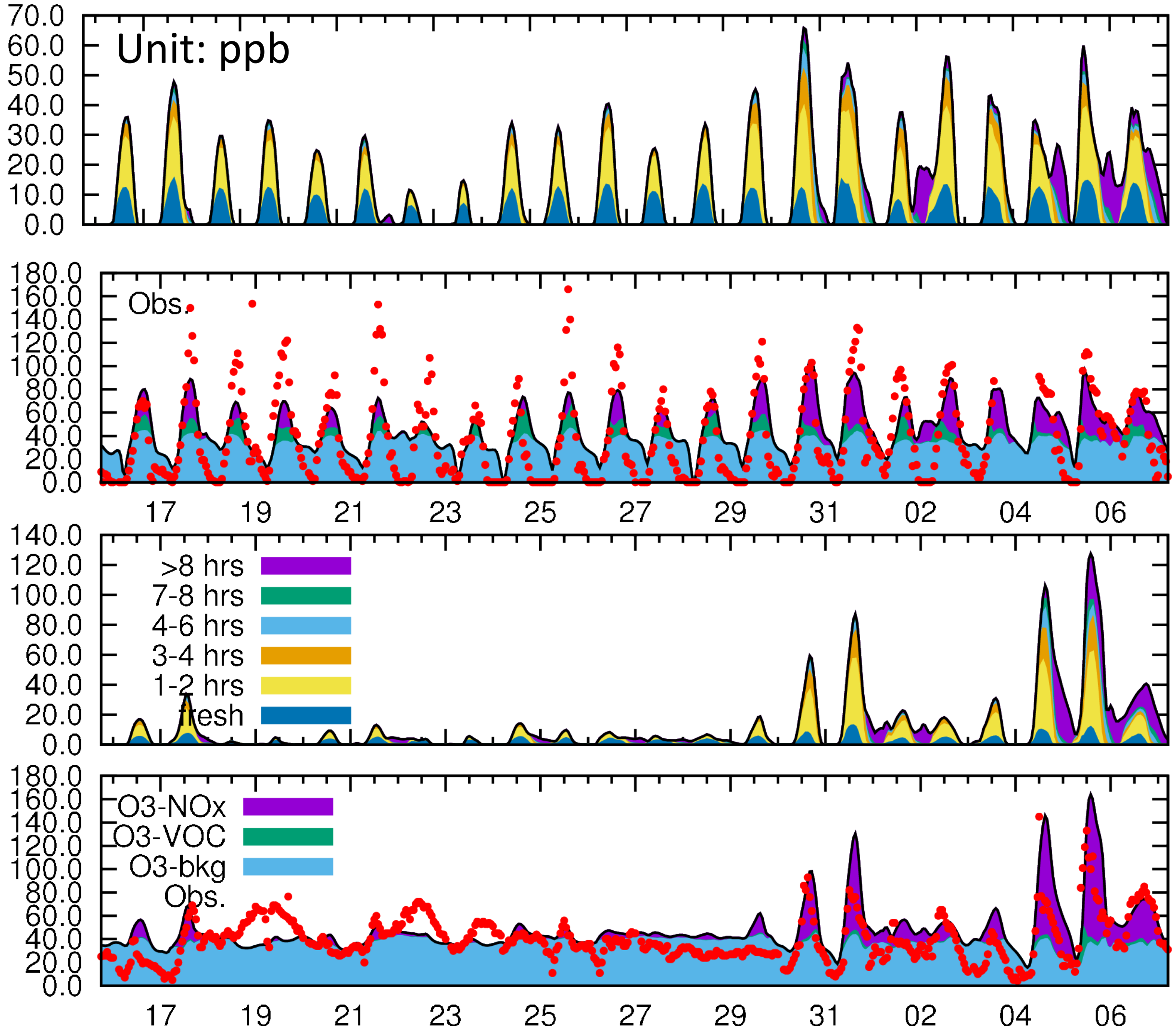
Model: CMAQ 5.0.1 + Condensed SAPRC07 with atmospheric aging/source/source region tracking

Aldine
Non-background O_3

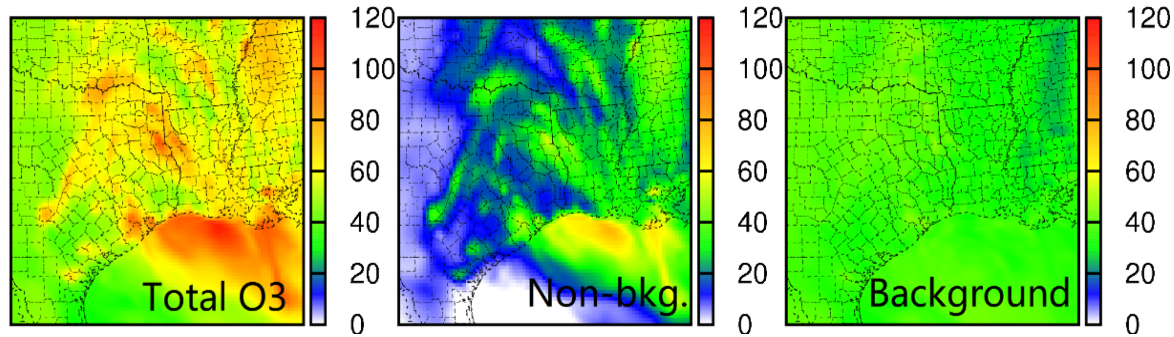
Aldine
Total O_3

Galveston
Non-background O_3

Galveston
Total O_3

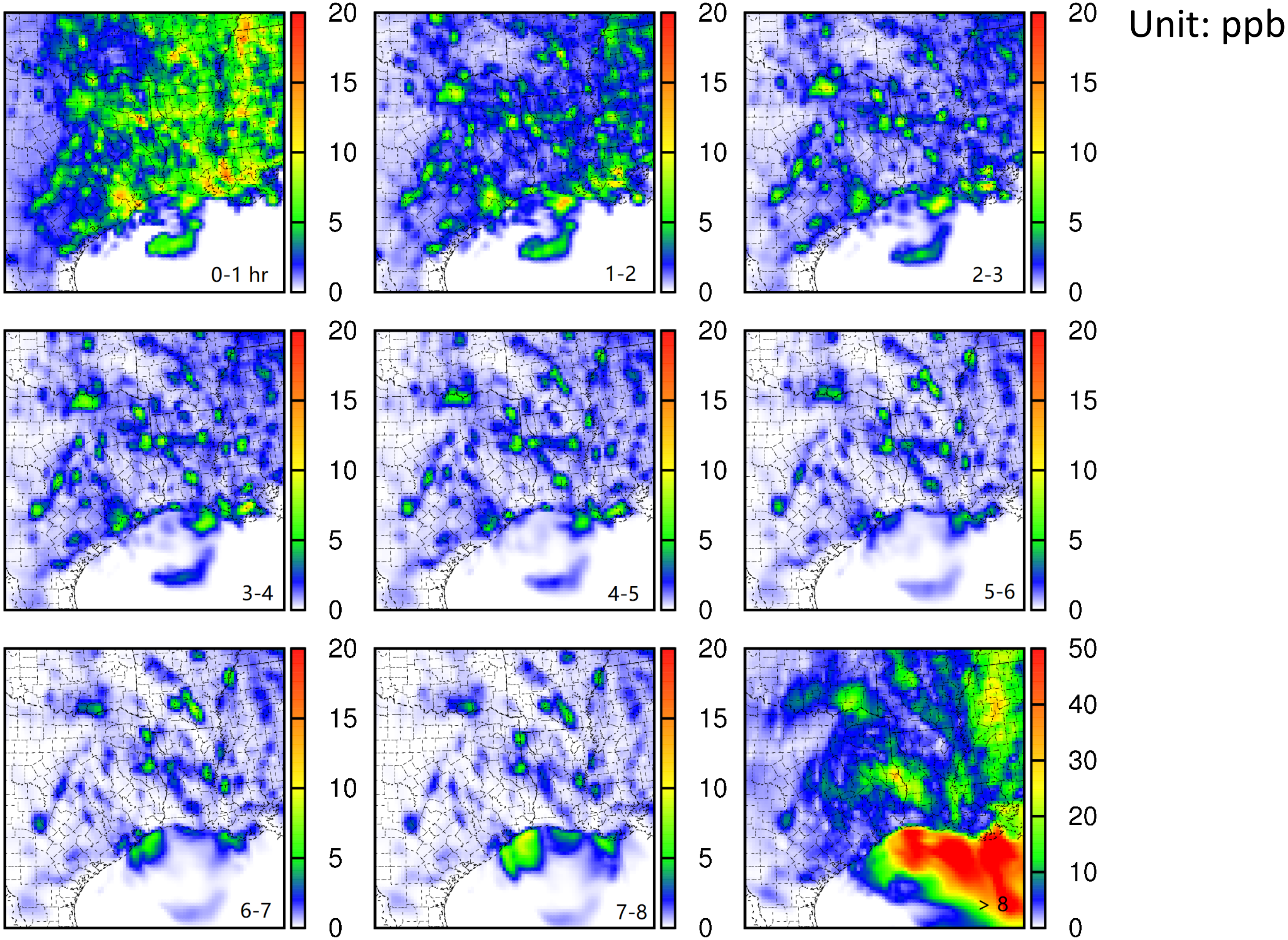


Regional distribution at 1500-1600 CST, August 30, 2000.



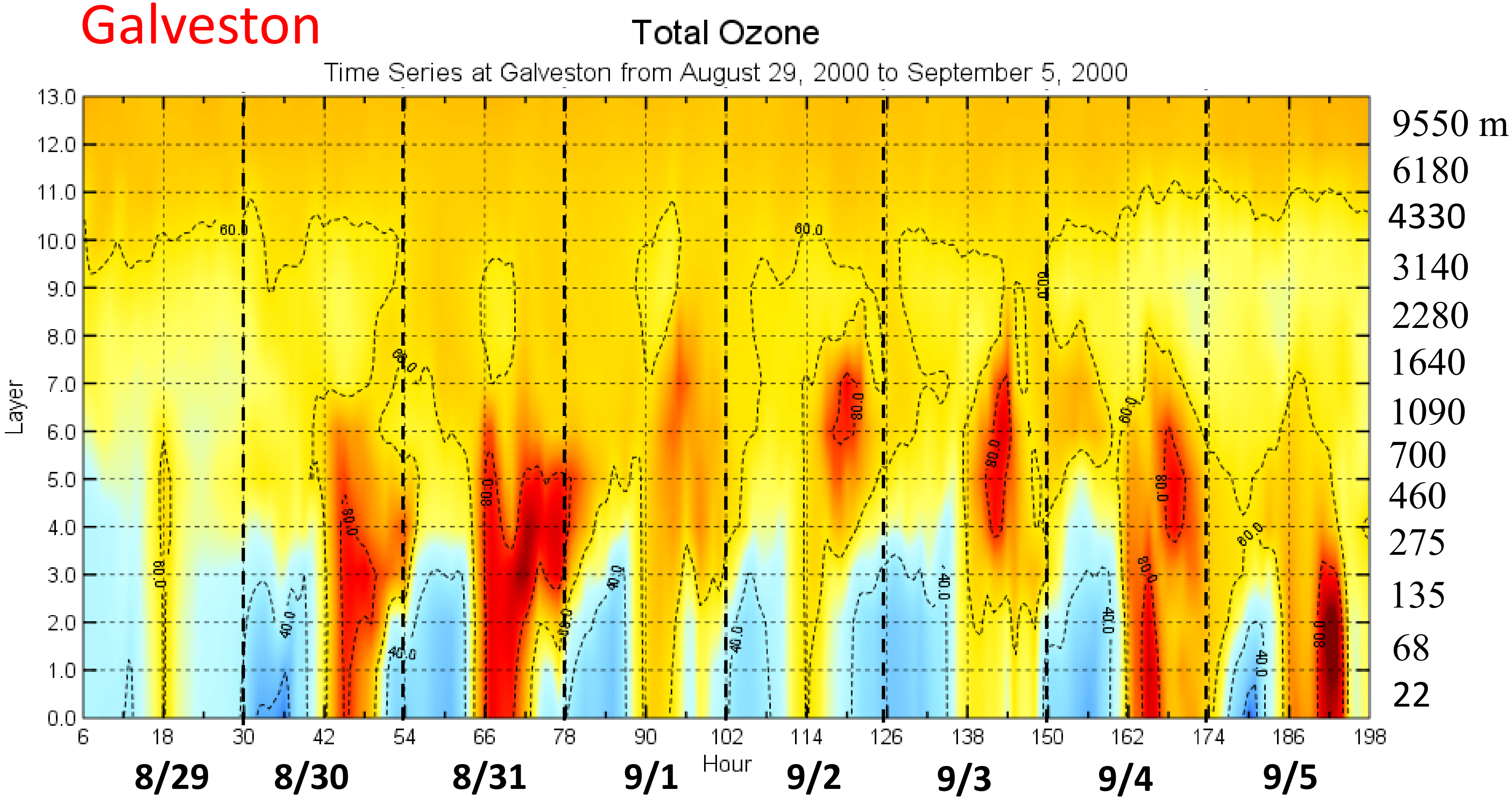
Regional age distribution of non-background ozone

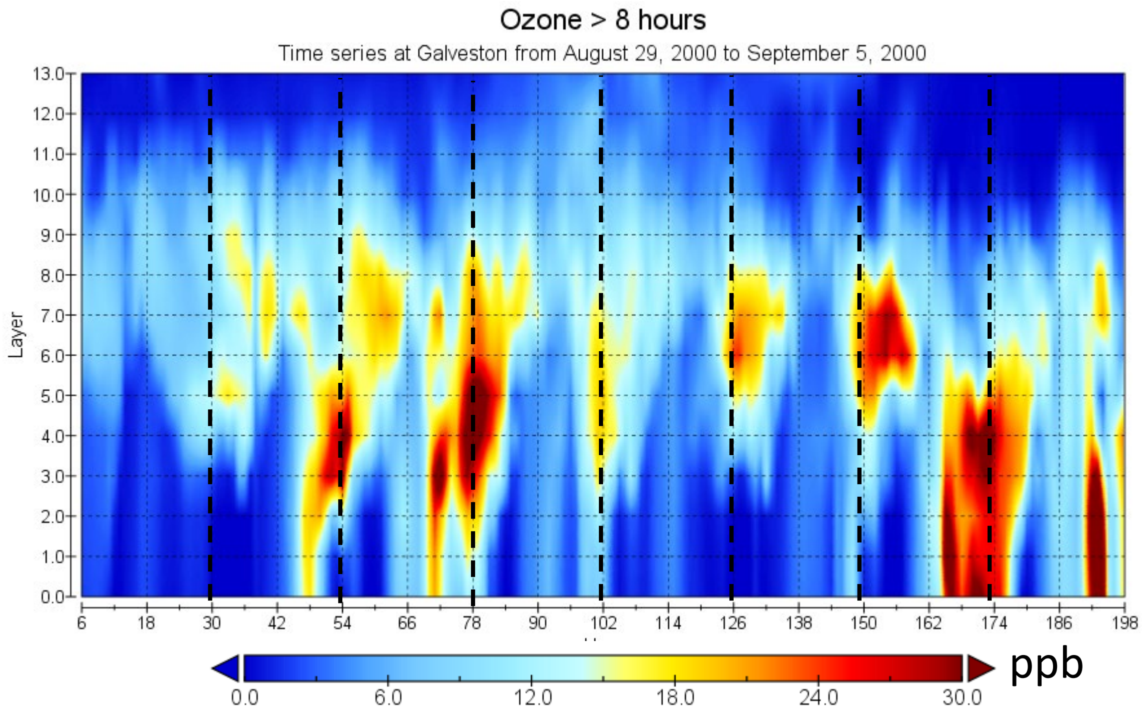
1500-1600 CST, August 30, 2000.



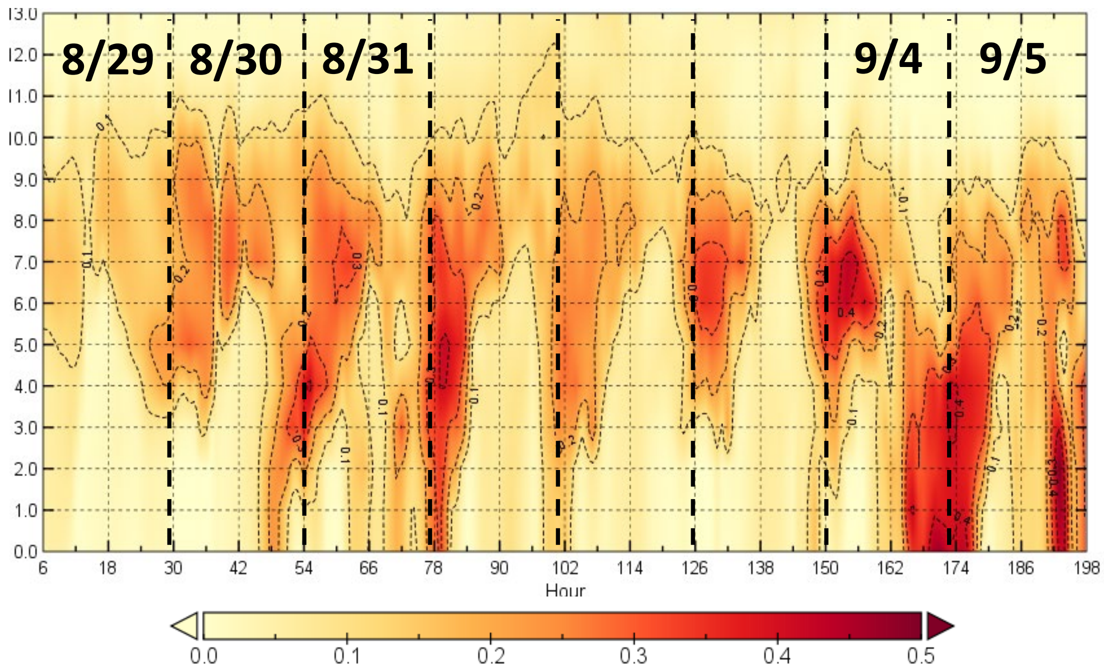
Vertical distribution of ozone – Total concentration

Galveston





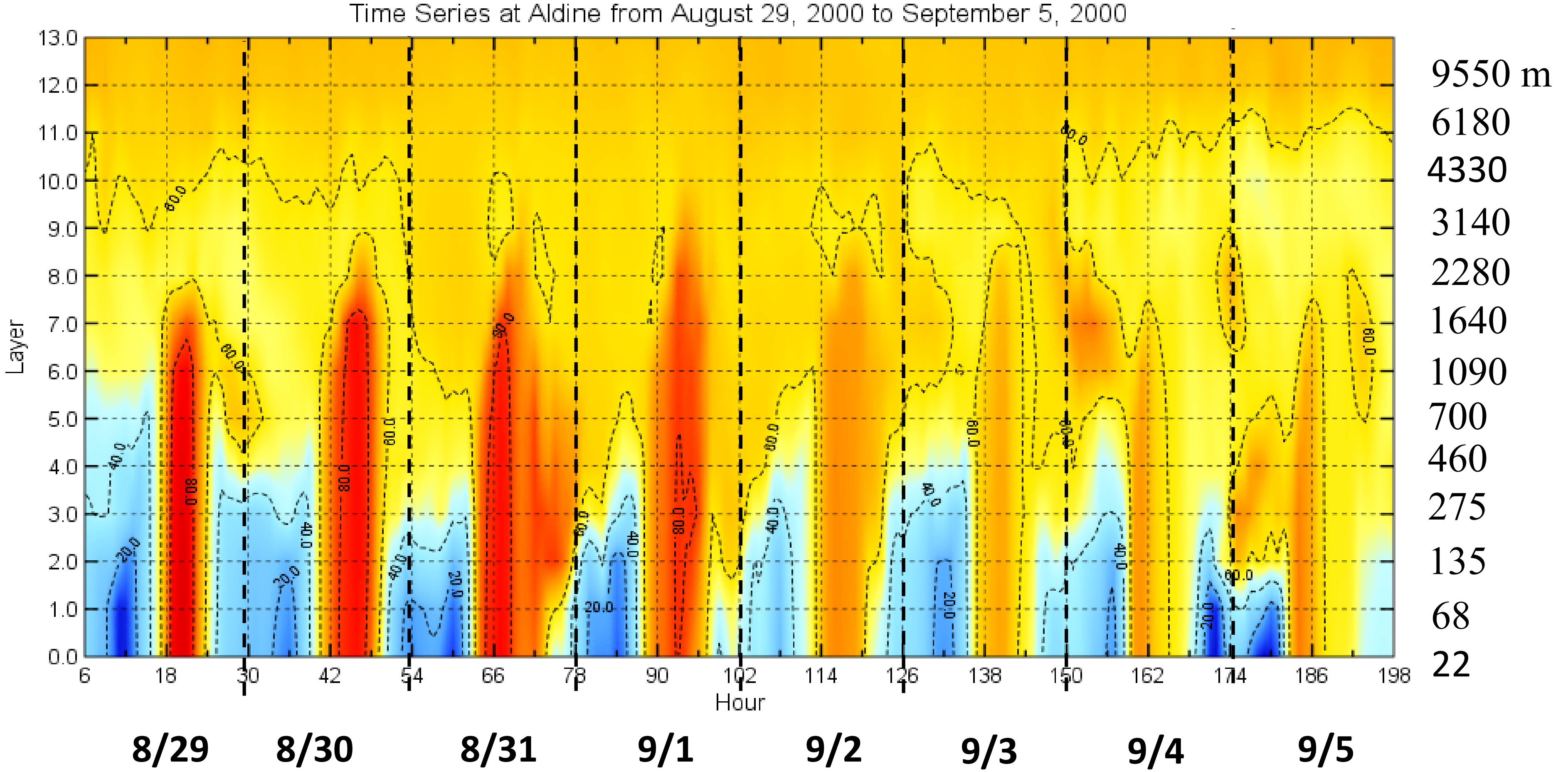
Aged Ozone (> 8 hrs)

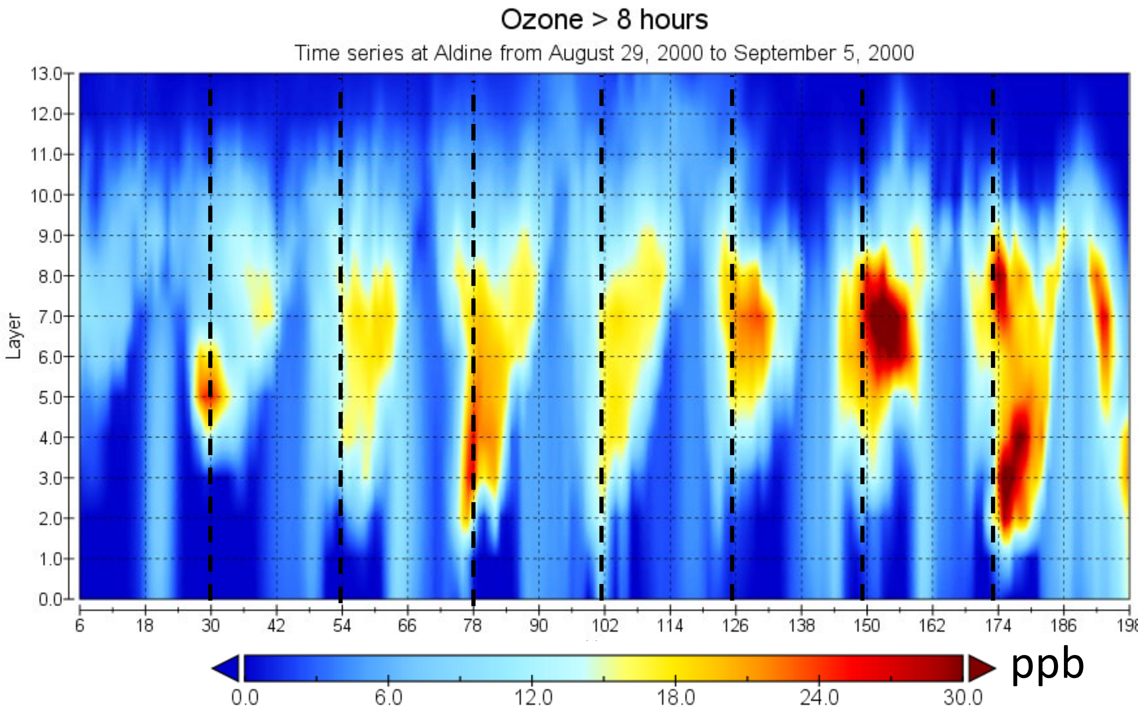


Fraction of aged ozone

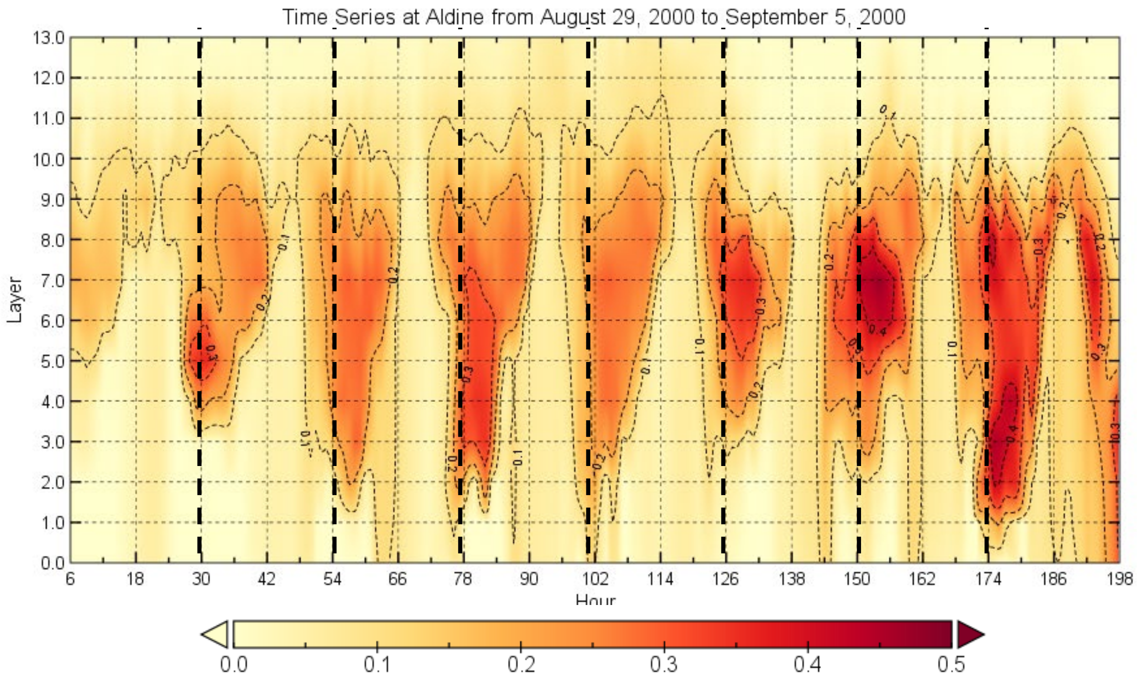
Vertical distribution of ozone – Total concentration

Aldine



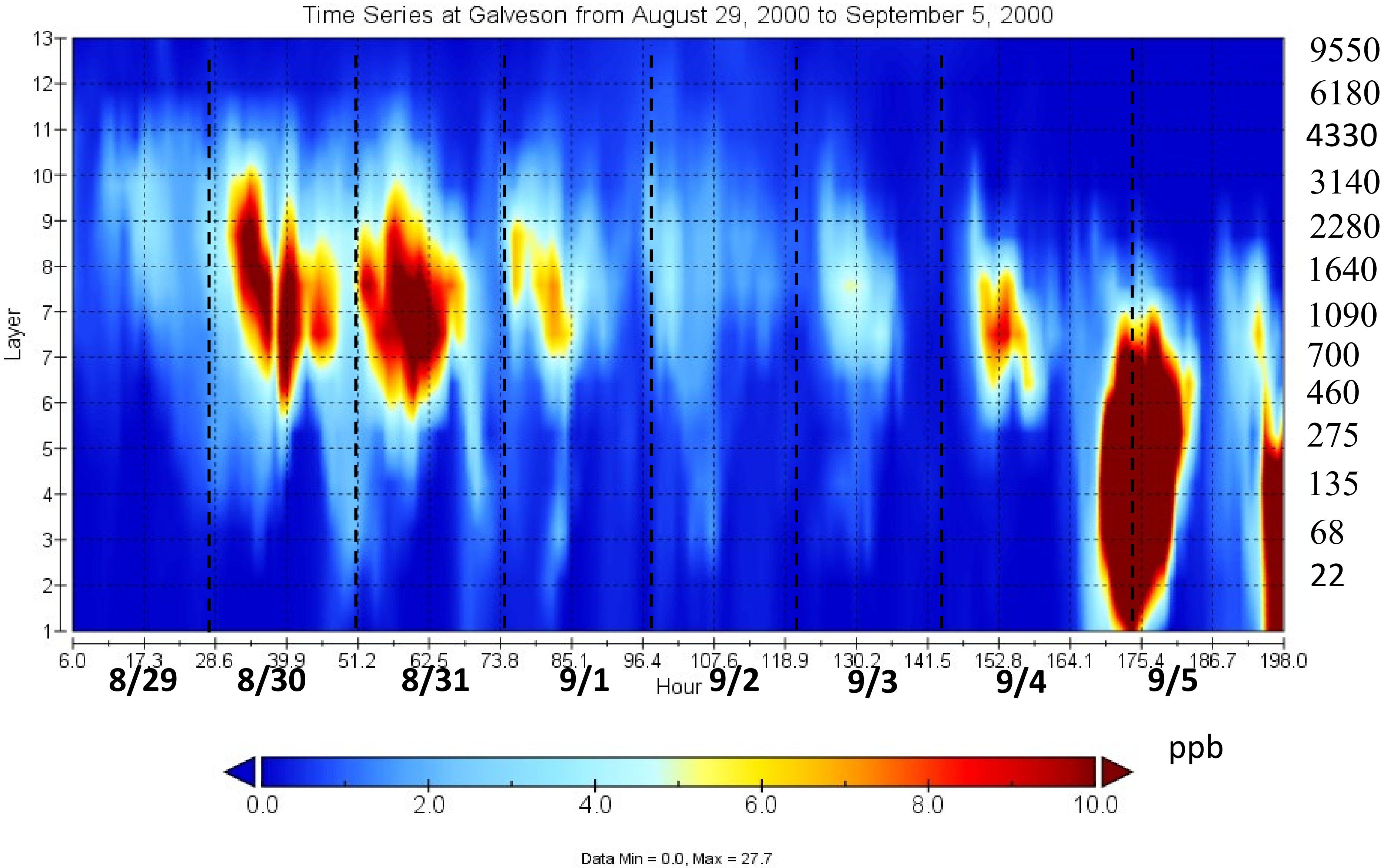


Aged Ozone (> 8 hrs)

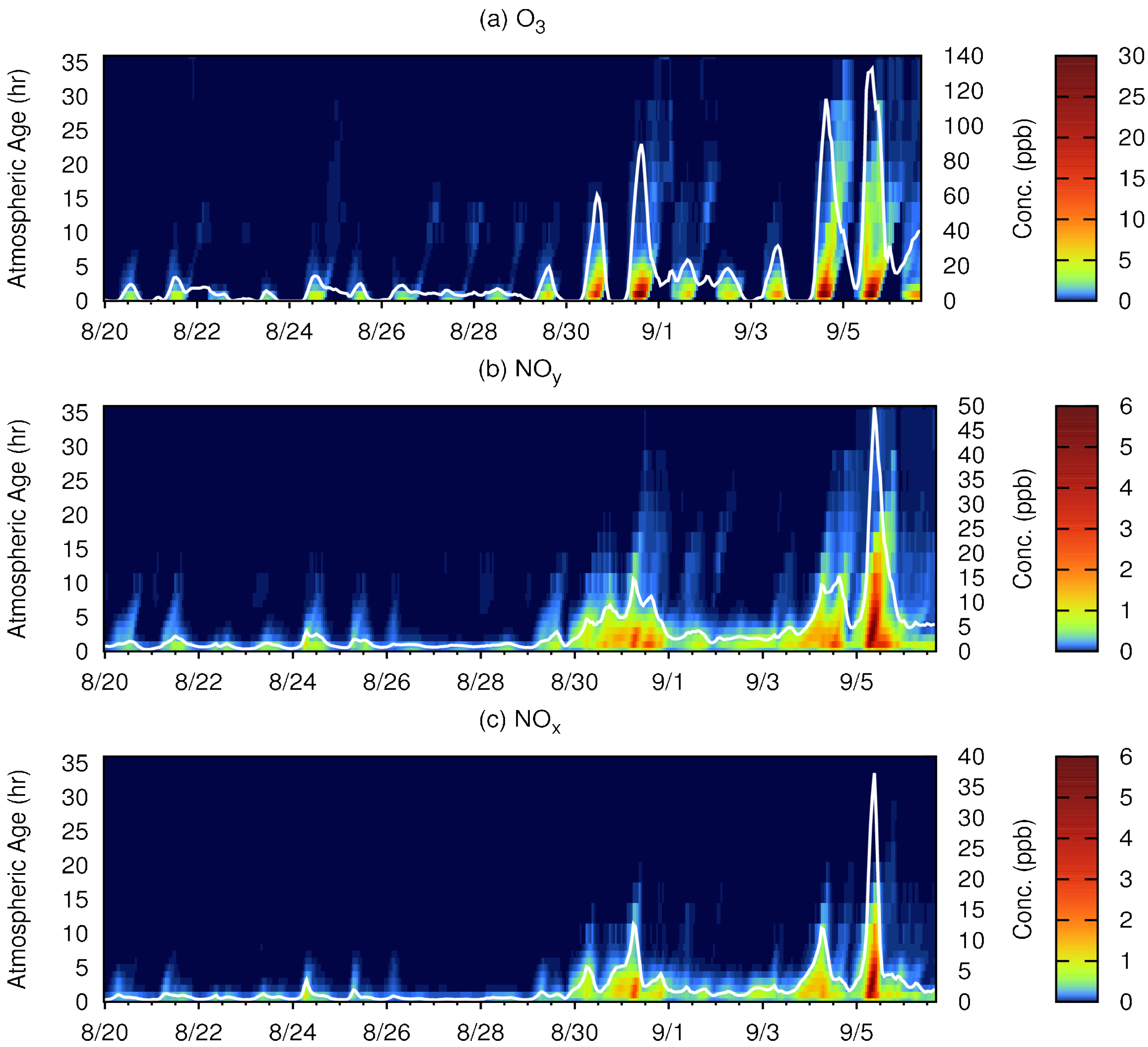


Fraction of aged ozone

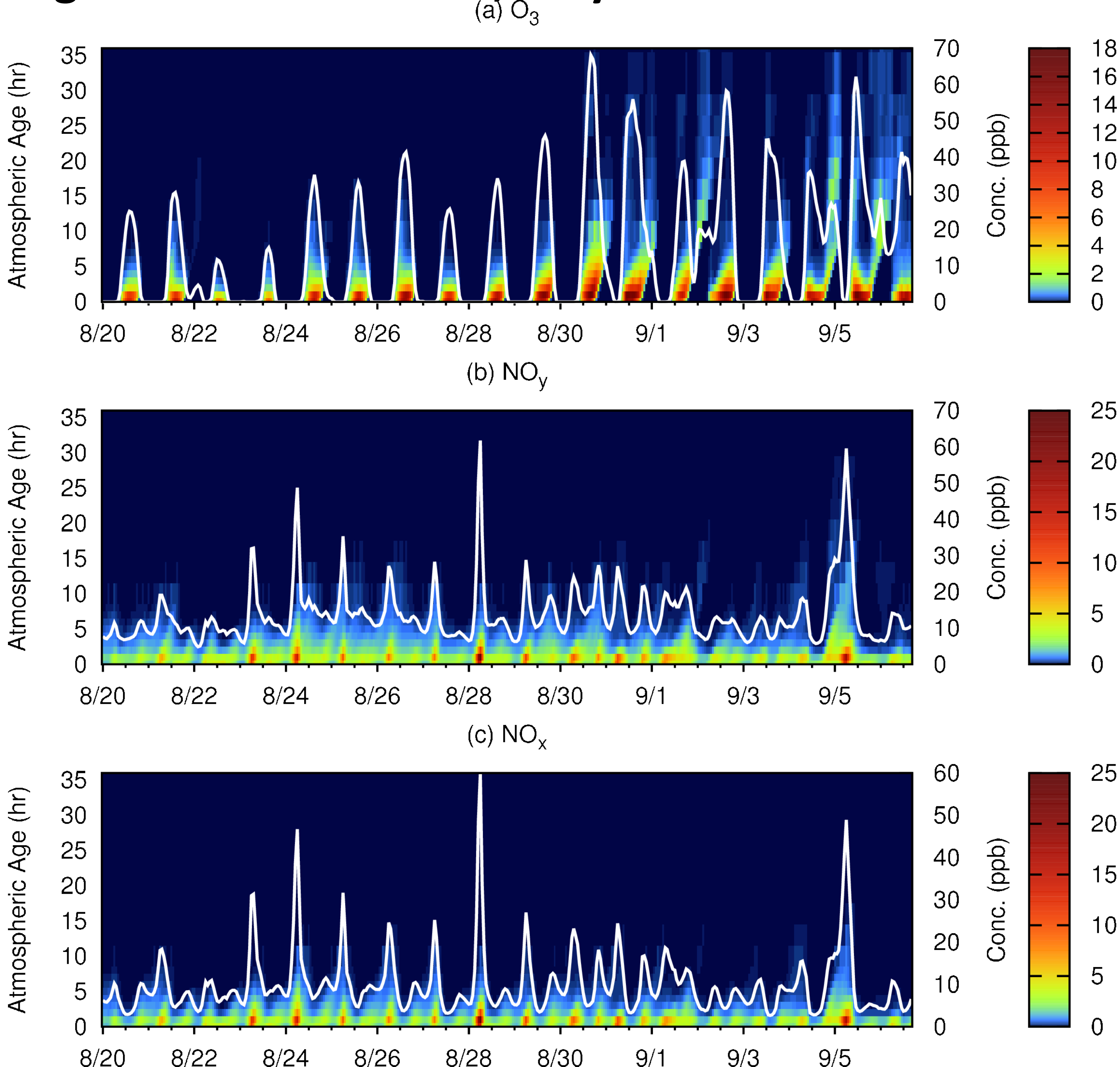
Galveston – O3 due to emissions from Louisiana



Age Distribution of O3, NOy and NOx at Galveston

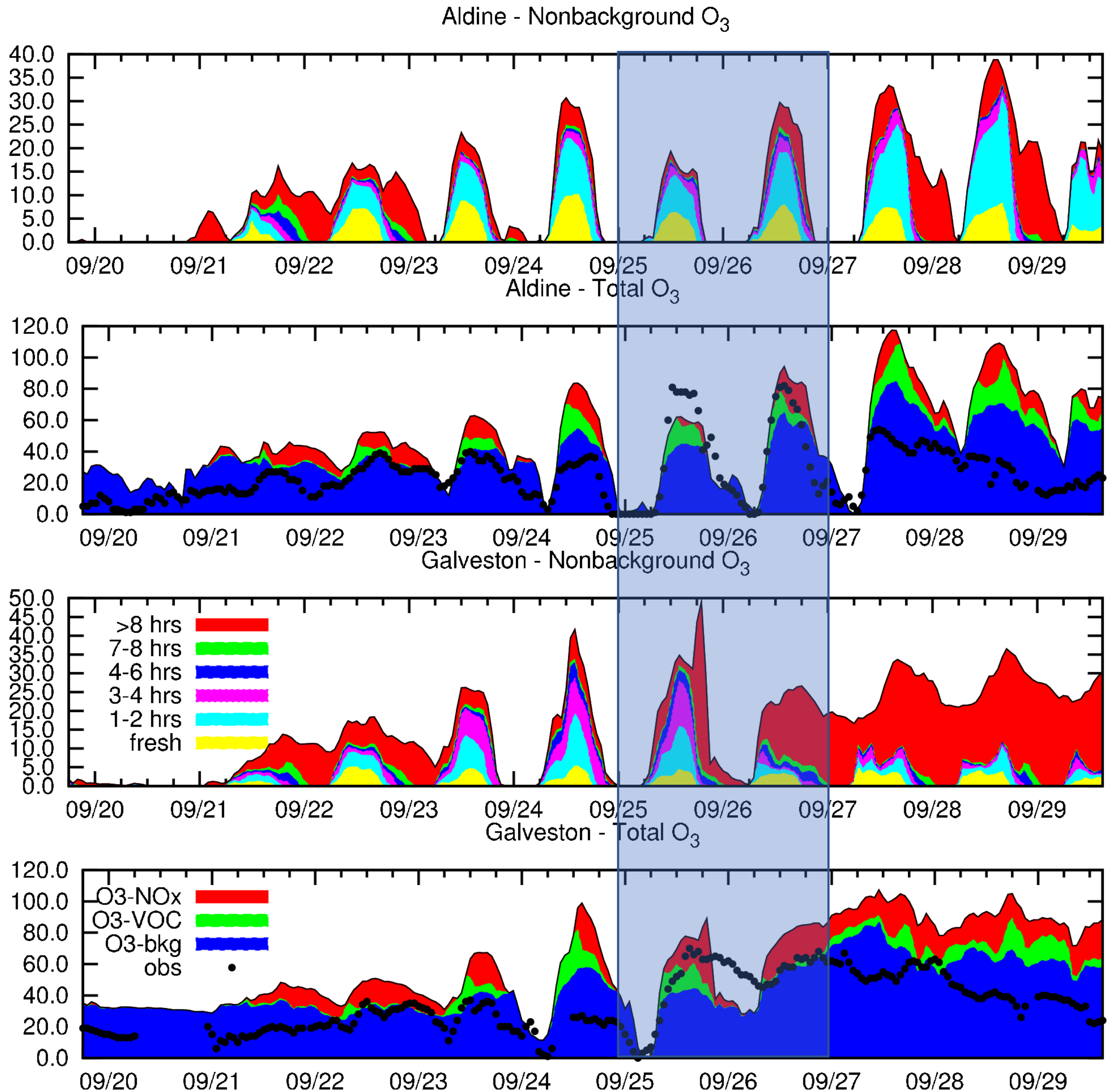


Age Distribution of O3, NOy and NOx at Aldine



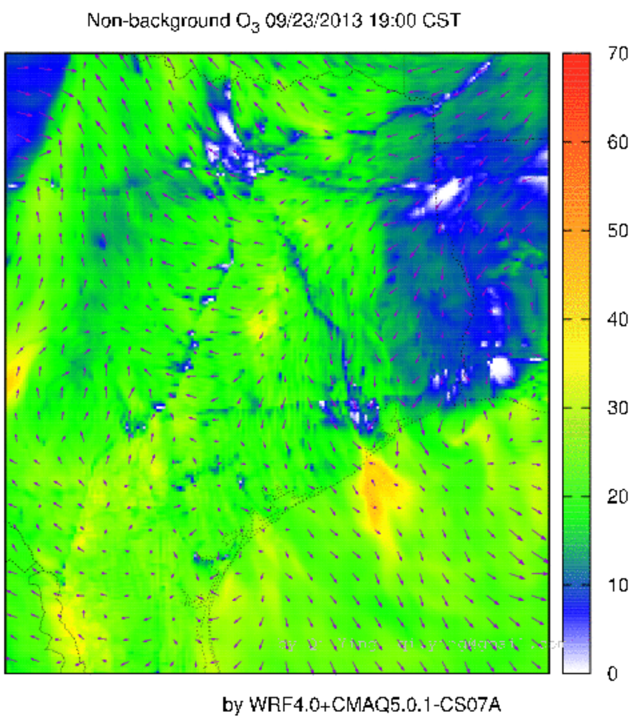
Case 2: September 2013 (DISCOVER-AQ)

September 25-26, 2013: The first day featured winds from the north, while the second day featured winds from the south. At low levels, the wind executed a complete clockwise loop during the day on September 25, while on September 26 the wind followed a classic moderate southerly wind pattern with variations in wind direction but no complete rotation.

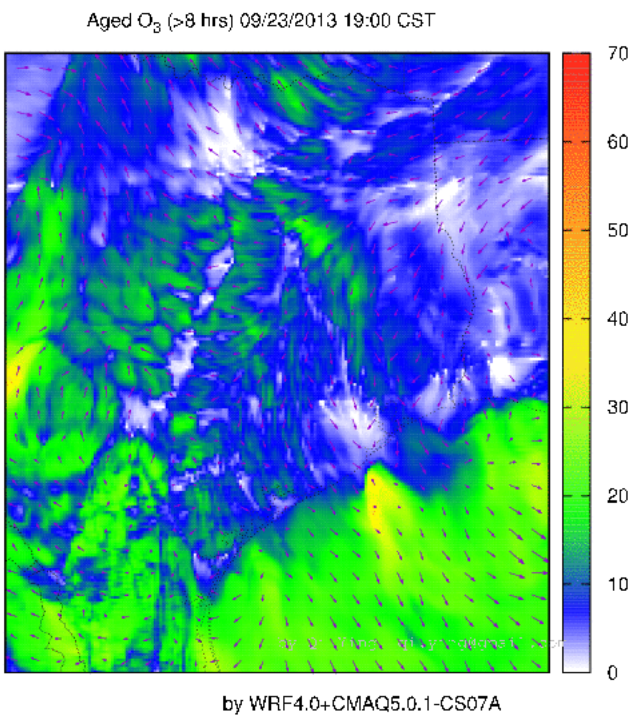


Aldine - Nonbackground O3
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
09/20
09/21
09/22
09/23
09/24
09/25
09/26
09/27
09/28
09/29
Aldine - Total O3
120.0
100.0
80.0
60.0
40.0
20.0
0.0
09/20
09/21
09/22
09/23
09/24
09/25
09/26
09/27
09/28
09/29
Galveston - Nonbackground O3
50.0
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
>8 hrs
7-8 hrs
4-6 hrs
3-4 hrs
1-2 hrs
fresh
09/20
09/21
09/22
09/23
09/24
09/25
09/26
09/27
09/28
09/29
Galveston - Total O3
120.0
100.0
80.0
60.0
40.0
20.0
0.0
O3-NOx
O3-VOC
O3-bkg
obs
09/20
09/21
09/22
09/23
09/24
09/25
09/26
09/27
09/28
09/29

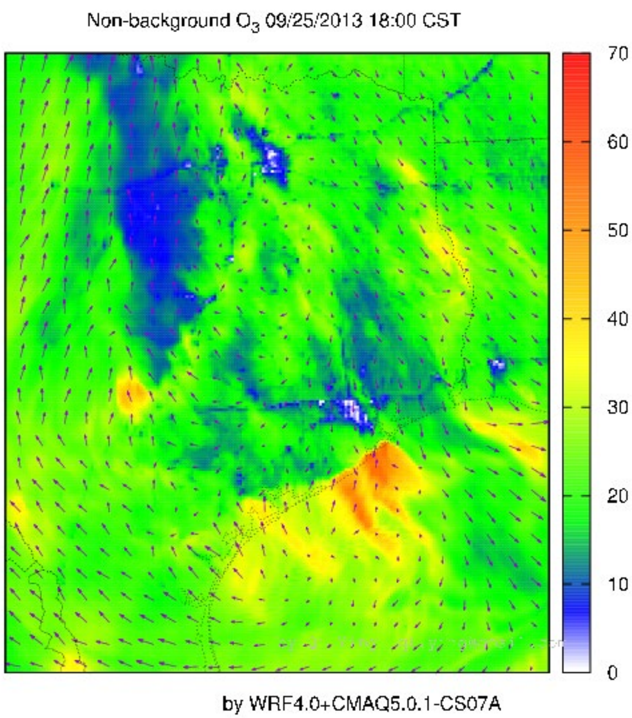
Non-Background Ozone

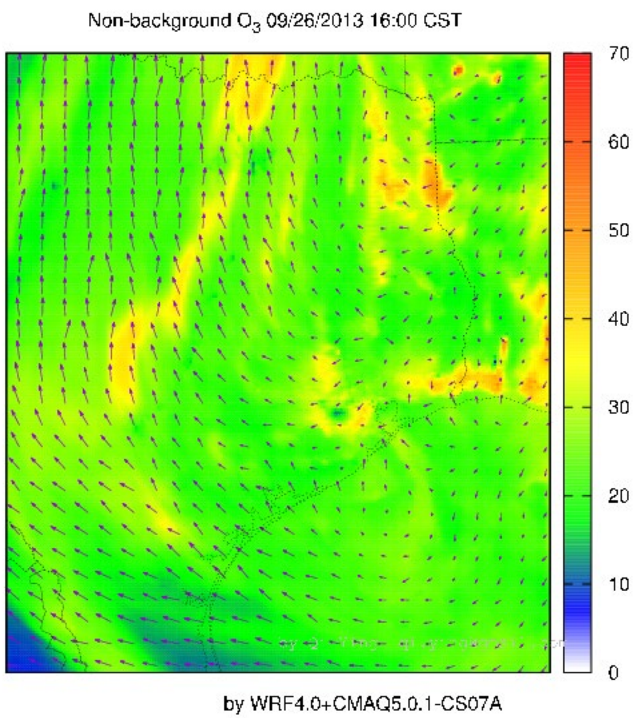


Aged Non-Background Ozone



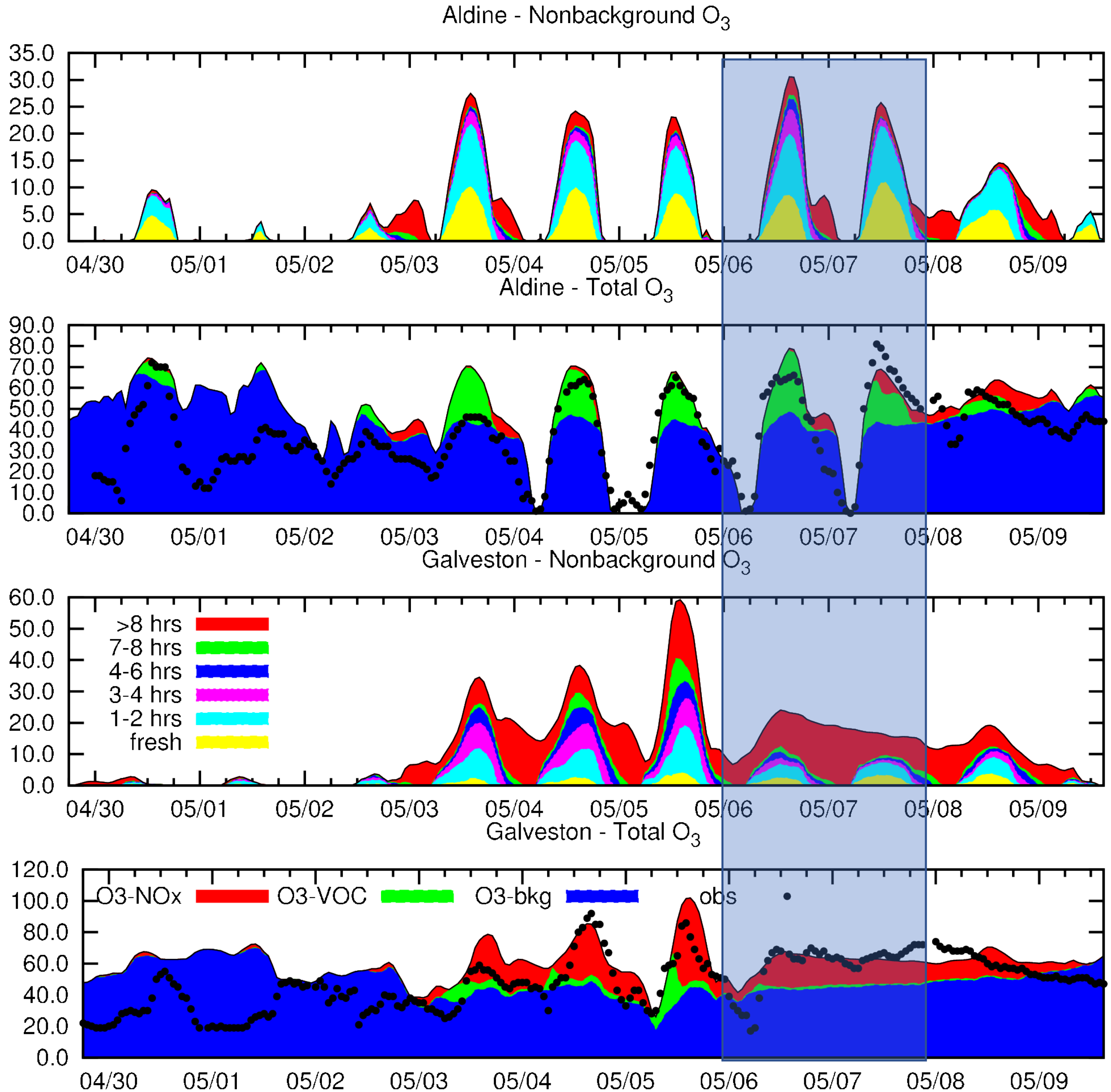
Snapshots, Sept 25-26, 2019





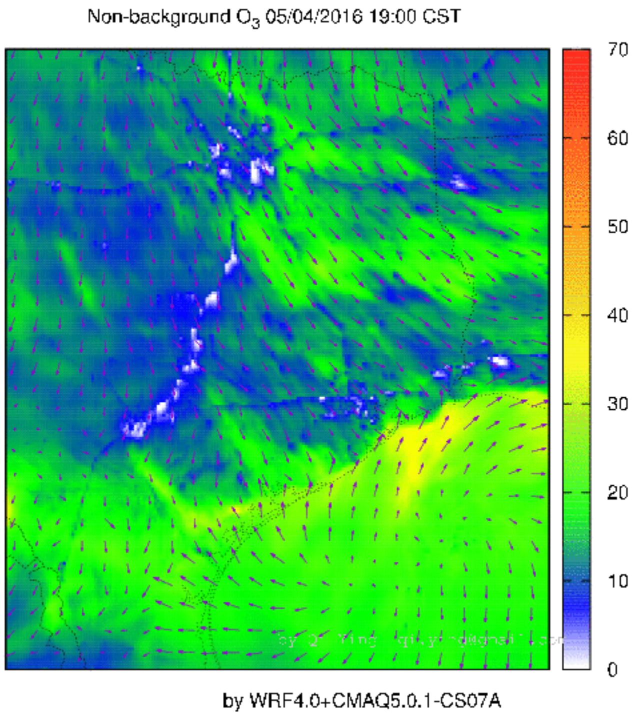
Case 3: May 6-7, 2016

A high vertical wind shear case, with low-level flow from the northeast and flow at 1800 m from the southwest. This case will be interesting because of that mix of different trajectories. Also the overall wind speed was unusually light on May 6, so the sea breeze circulation should be easier to detect. This case will test the ability of the model to properly represent pure thermally-forced boundary layer circulations.

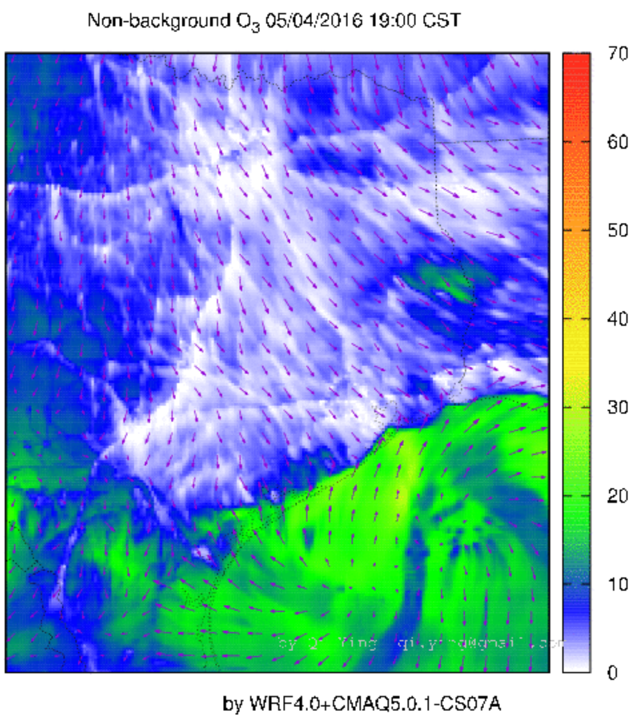


Aldine - Nonbackground O_3
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
04/30
05/01
05/02
05/03
05/04
05/05
05/06
05/07
05/08
05/09
Aldine - Total O_3
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
Galveston - Nonbackground O_3
60.0
50.0
40.0
30.0
20.0
10.0
0.0
>8 hrs
7-8 hrs
4-6 hrs
3-4 hrs
1-2 hrs
fresh
Galveston - Total O_3
120.0
100.0
80.0
60.0
40.0
20.0
0.0
O3-NOx
O3-VOC
O3-bkg
obs

Non-Background Ozone

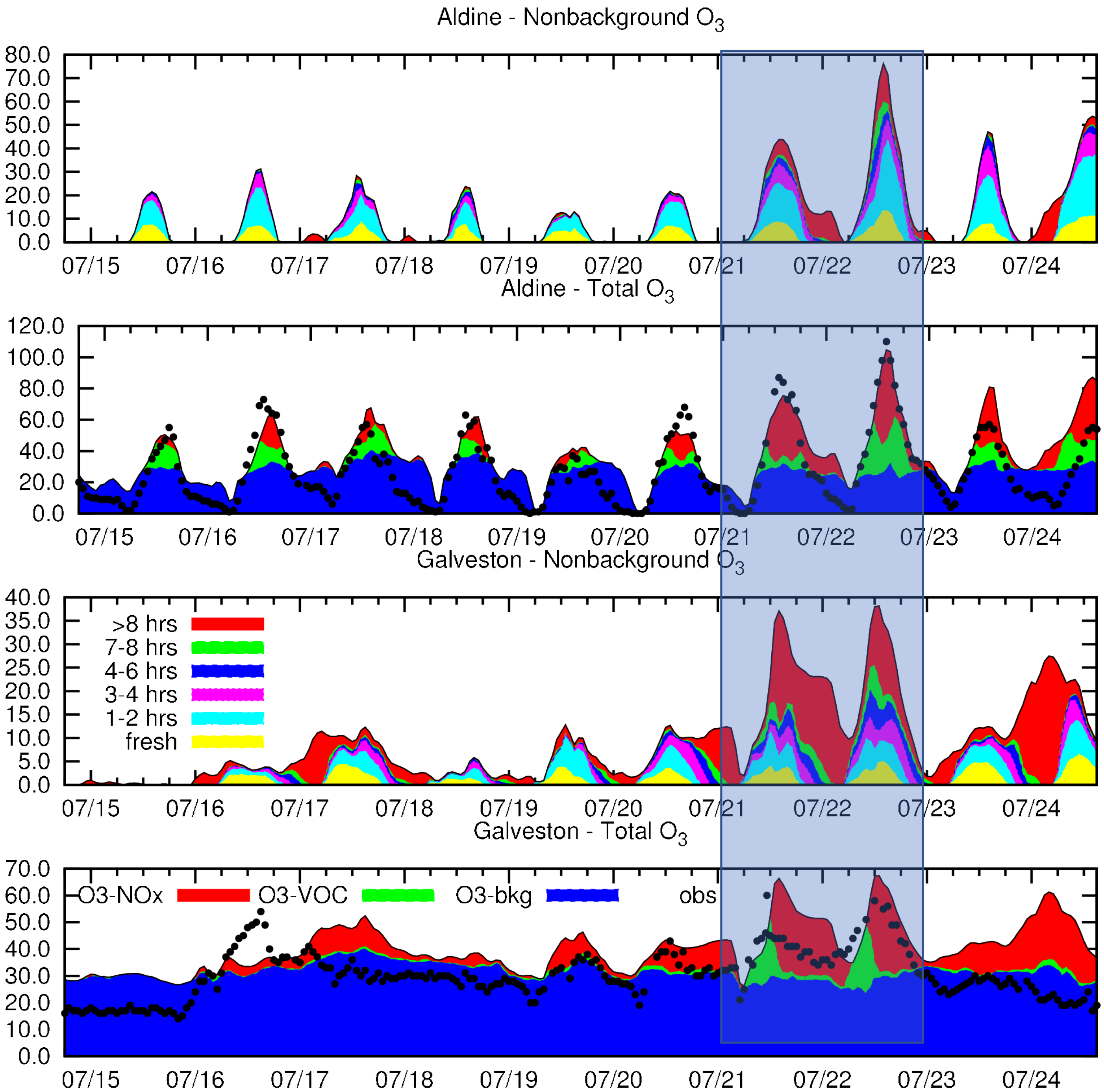


Aged Non-Background Ozone

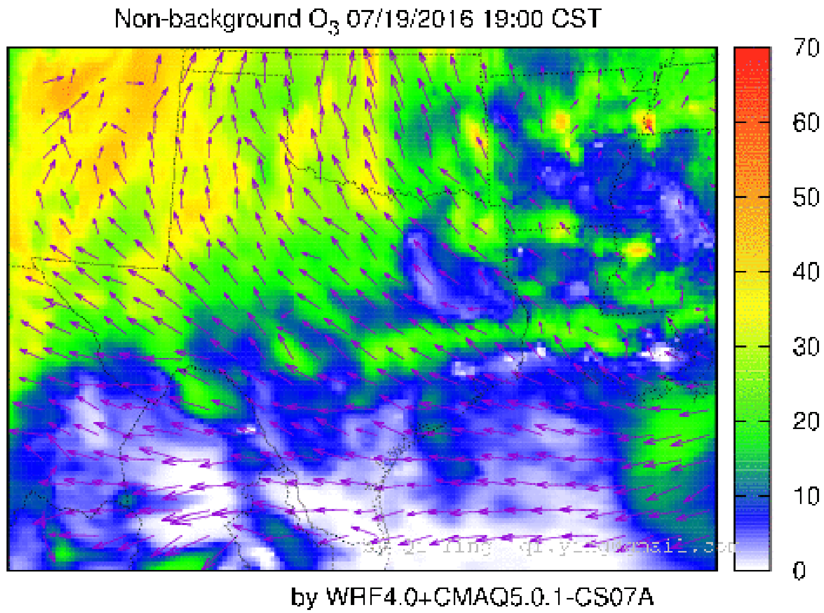


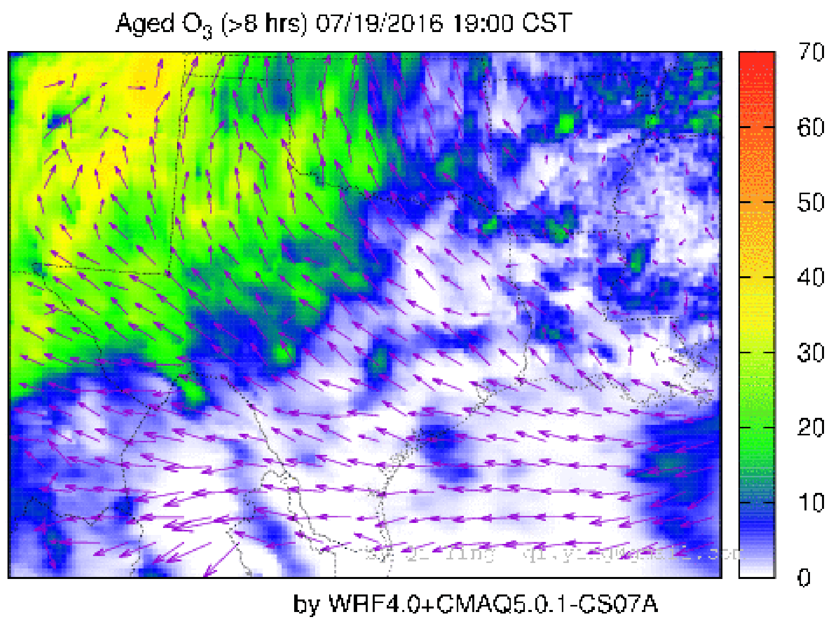
Case 4: July 21-22, 2016

A classic sea breeze case, with flow from the east or southeast at all levels. Low-level winds do complete rotations.

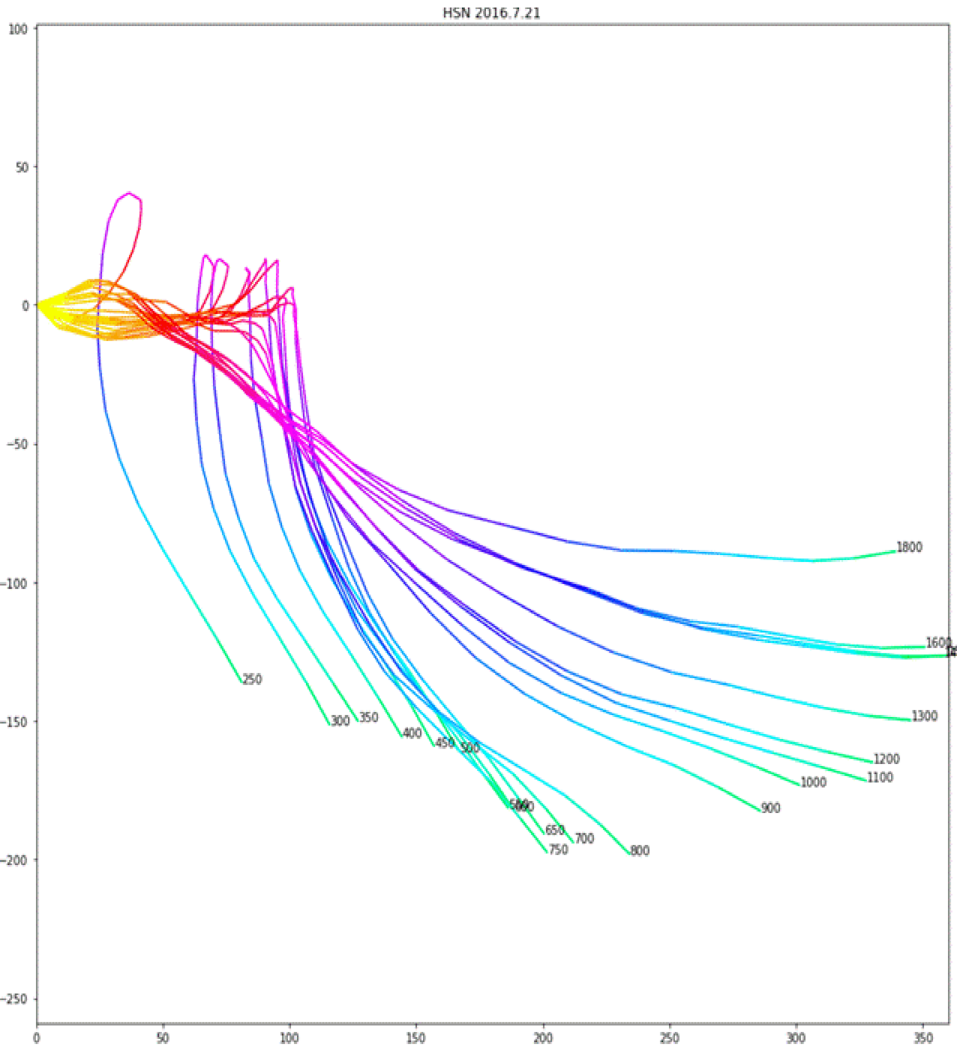


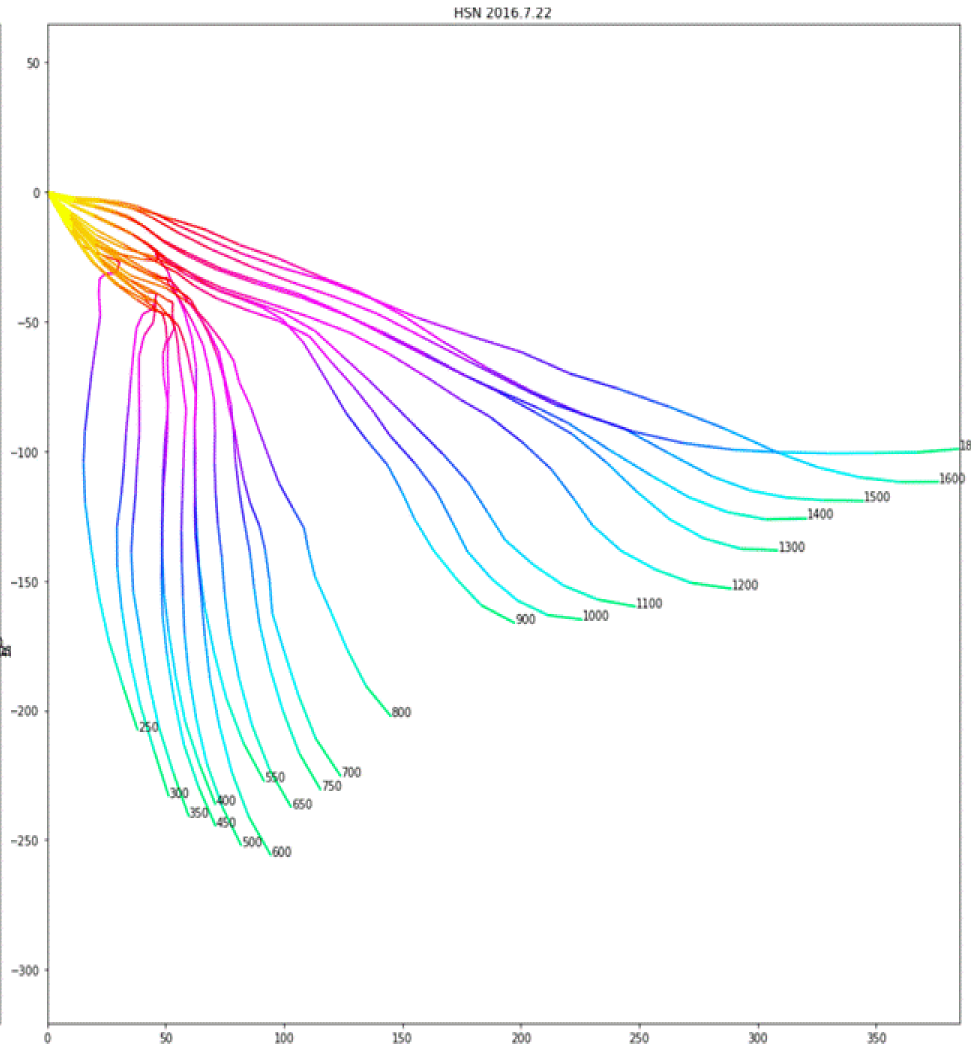
Aldine - Nonbackground O_3
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
07/15 07/16 07/17 07/18 07/19 07/20 07/21 07/22 07/23 07/24
Aldine - Total O_3
120.0
100.0
80.0
60.0
40.0
20.0
0.0
07/15 07/16 07/17 07/18 07/19 07/20 07/21 07/22 07/23 07/24
Galveston - Nonbackground O_3
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
>8 hrs
7-8 hrs
4-6 hrs
3-4 hrs
1-2 hrs
fresh
07/15 07/16 07/17 07/18 07/19 07/20 07/21 07/22 07/23 07/24
Galveston - Total O_3
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
O3-NOx
O3-VOC
O3-bkg
obs
07/15 07/16 07/17 07/18 07/19 07/20 07/21 07/22 07/23 07/24

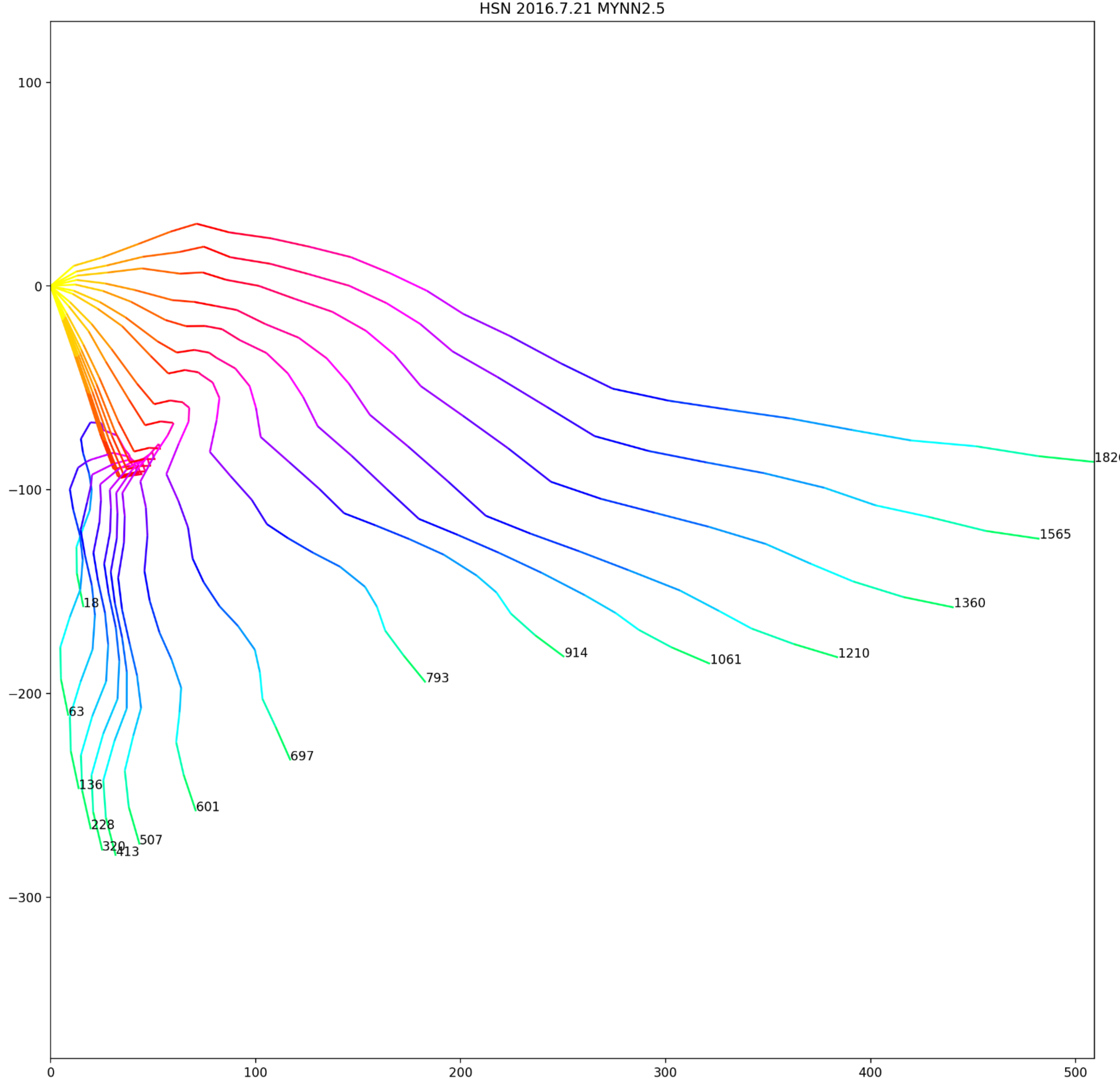

Non-background O_3 07/19/2016 19:00 CST
70
60
50
40
30
20
10
0
by WRF4.0+CMAQ5.0.1-CS07A

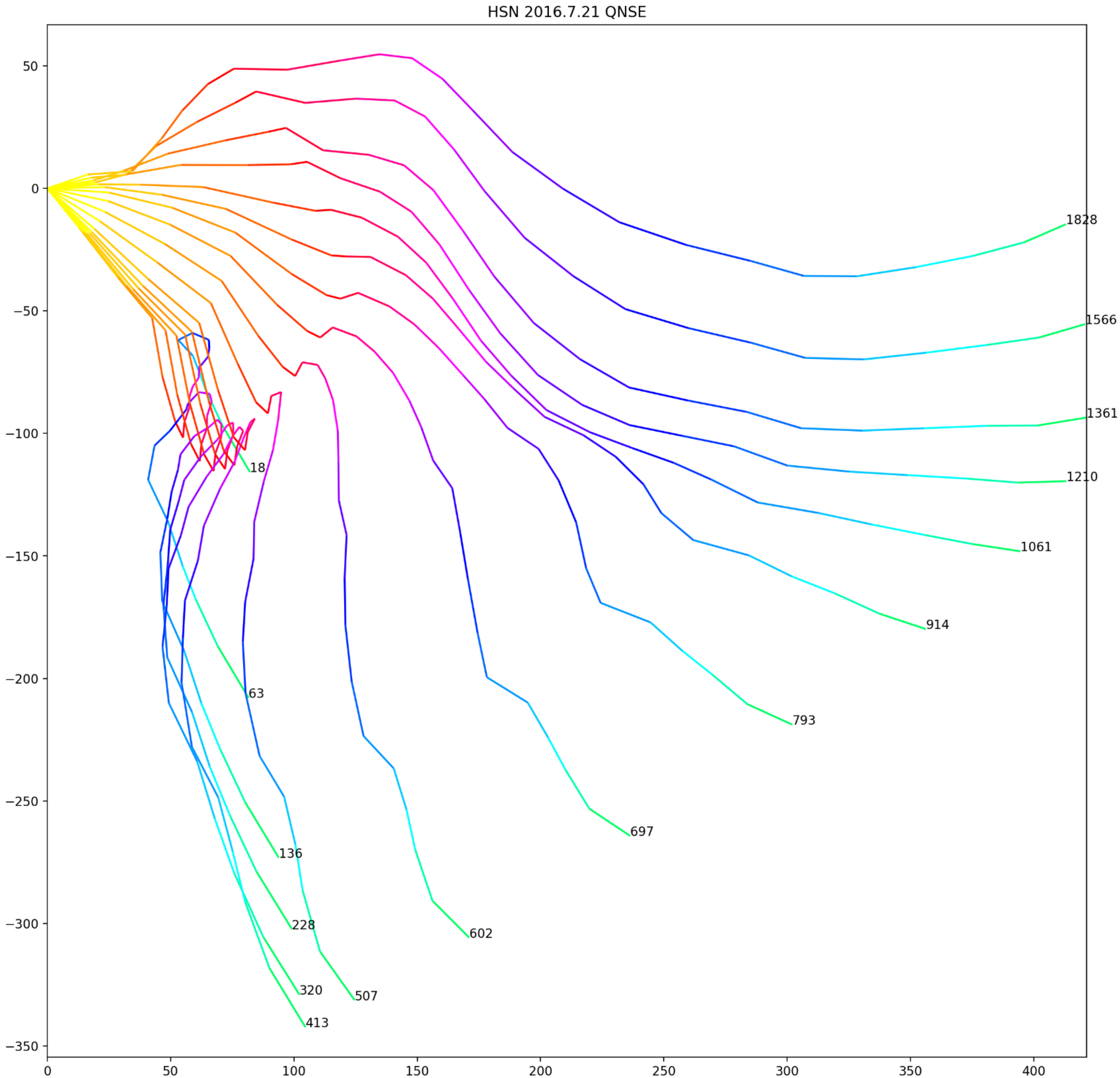

Aged O_3 (>8 hrs) 07/19/2016 19:00 CST
70
60
50
40
30
20
10
0
by WRF4.0+CMAQ5.0.1-CS07A

July 2016 case: July 21-22

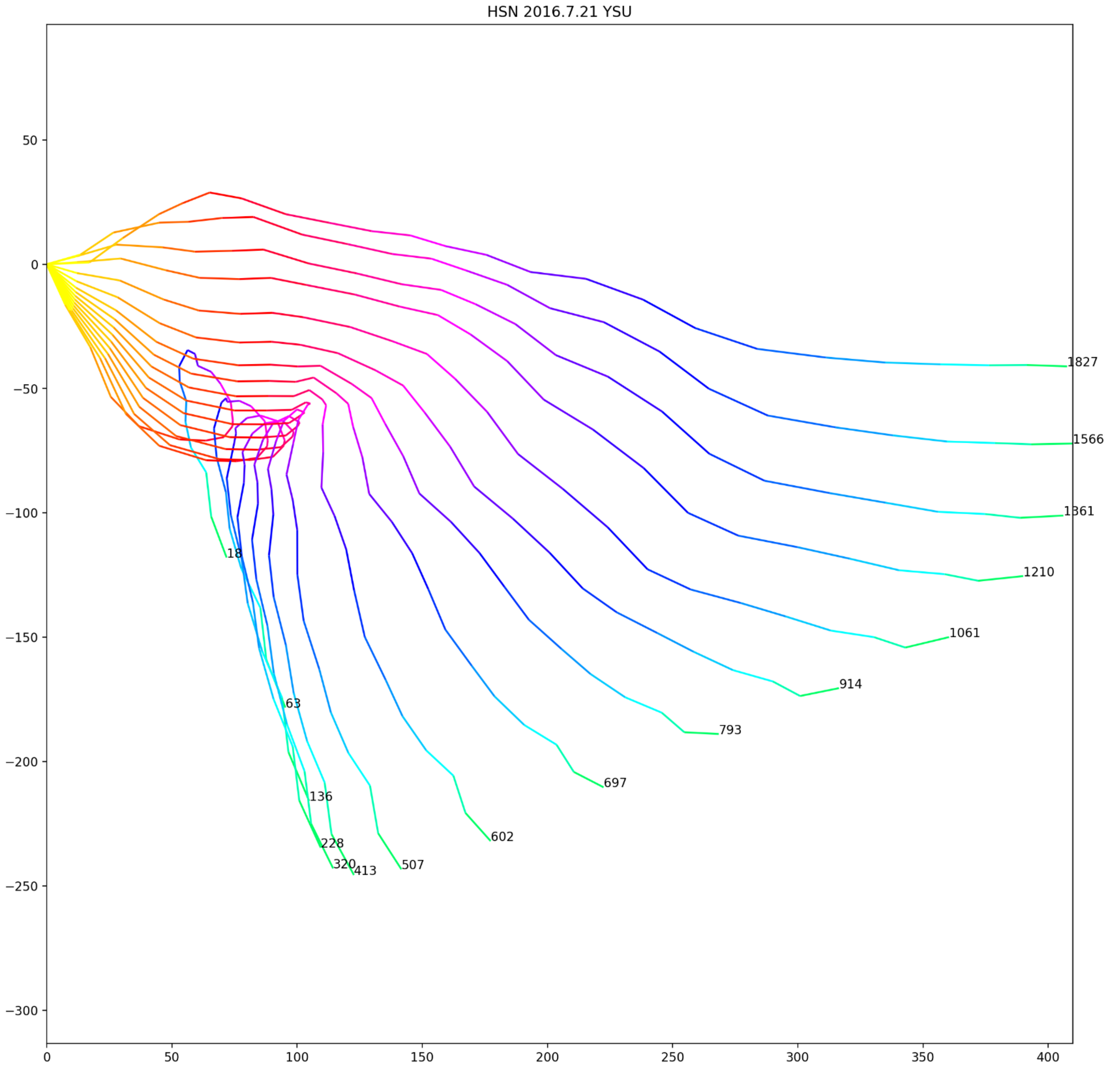


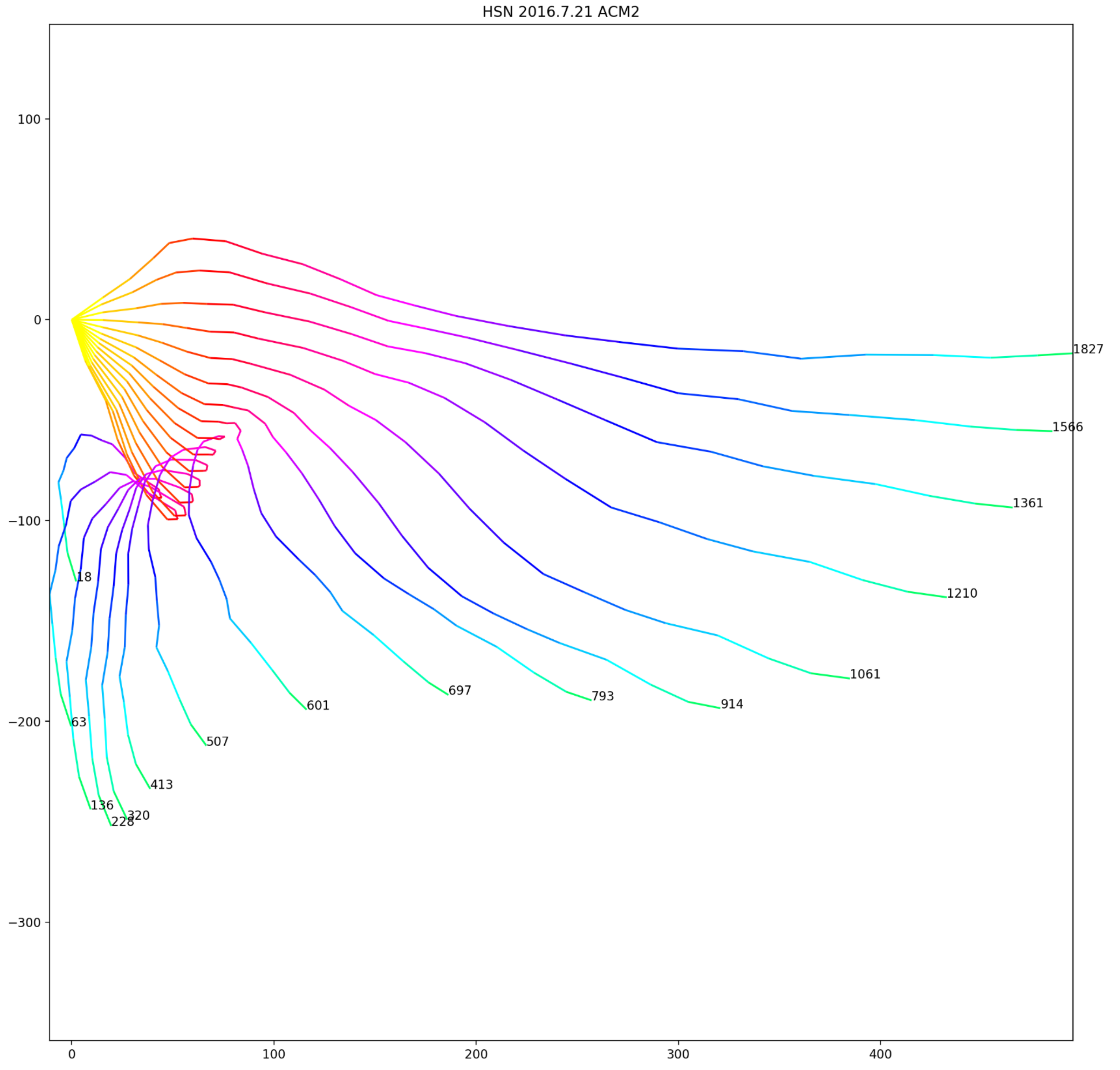



HSN 2016.7.21 MYNN2.5
100
0
−100
−200
−300
0
100
200
300
400
500
1826
1565
1360
1210
1061
914
793
697
601
507
413
320
228
136
63
18

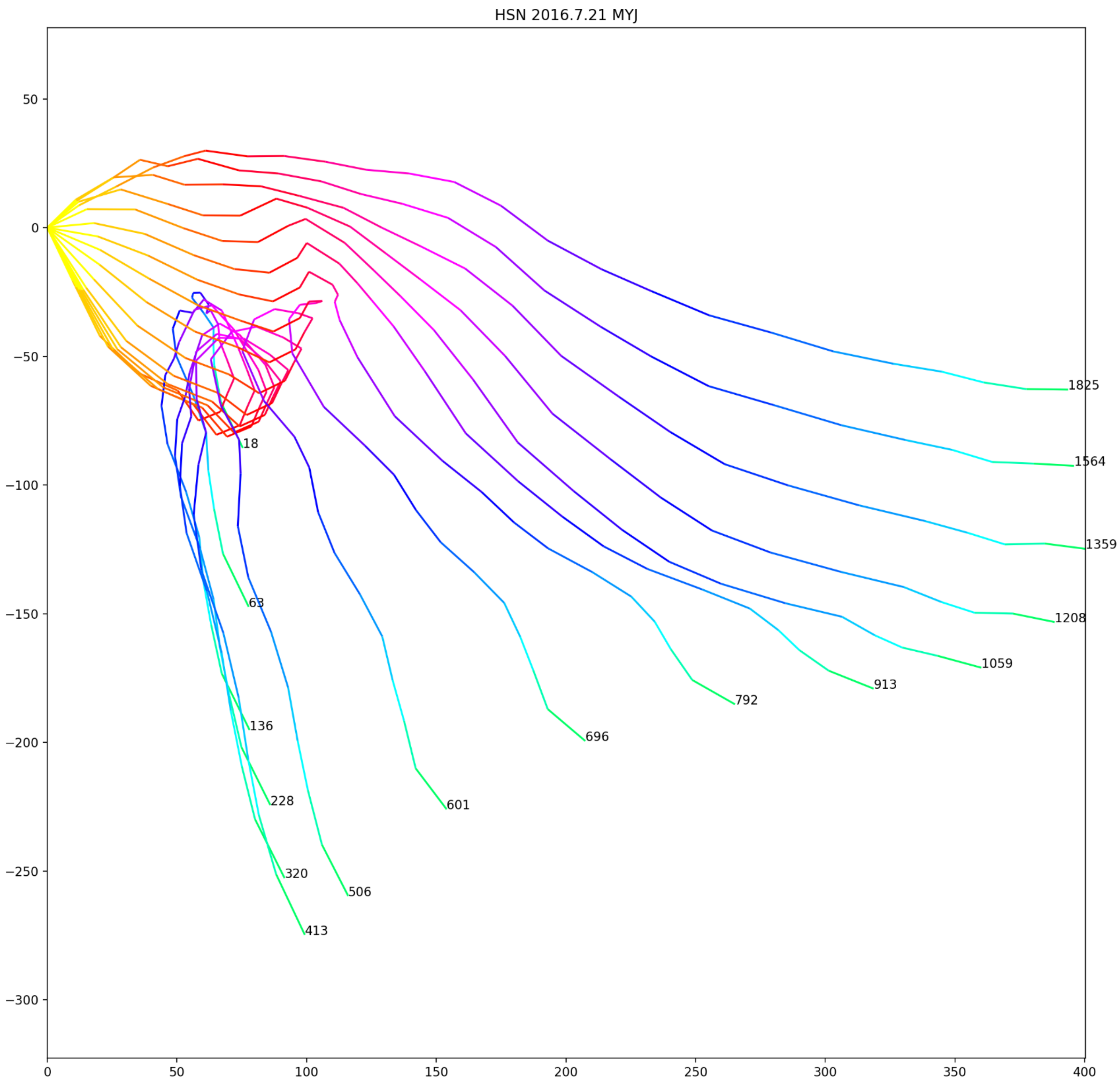


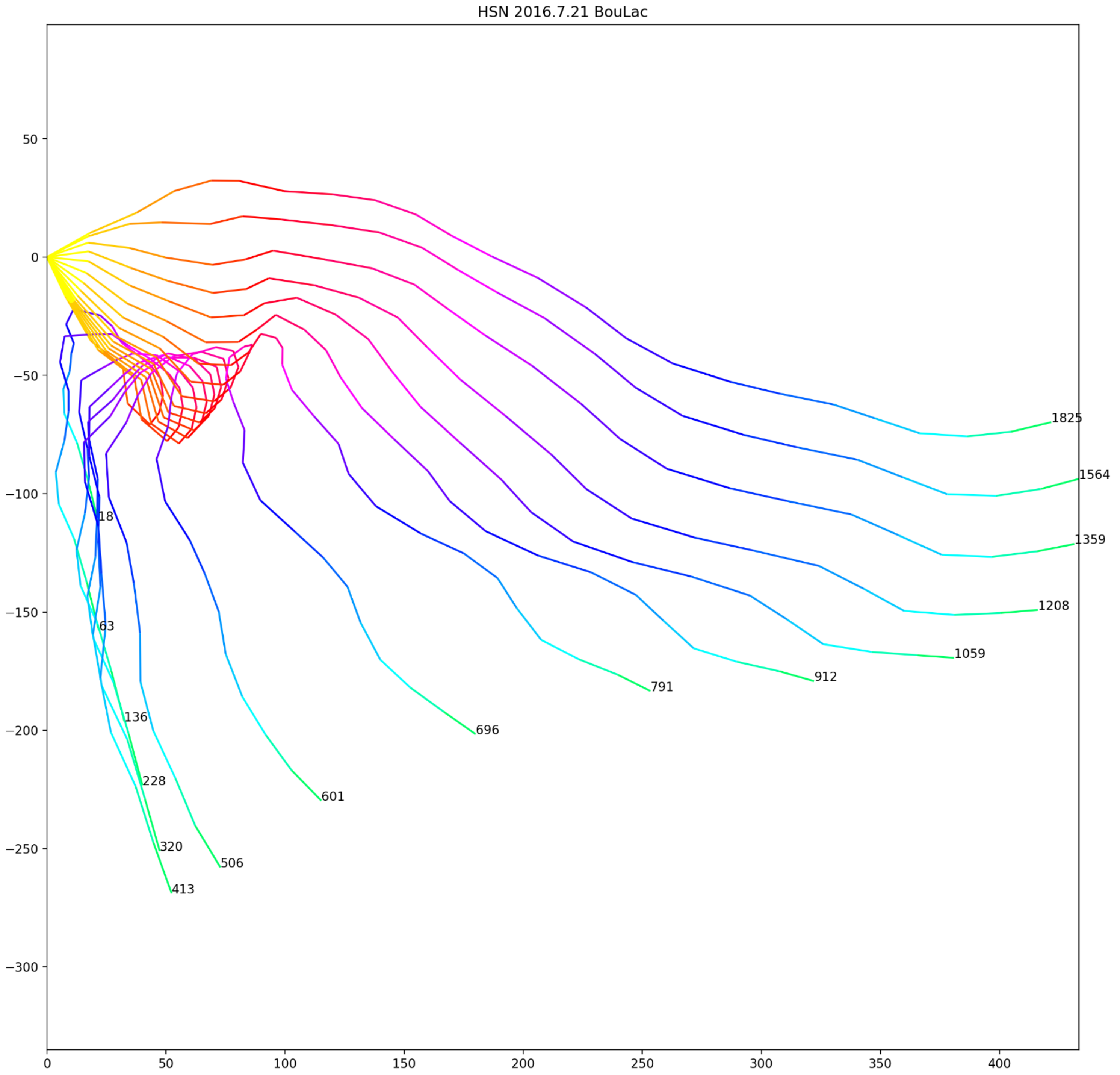
HSN 2016.7.21 QNSE
1828
1566
1361
1210
1061
914
793
697
602
507
413
320
228
136
63
18
50
0
−50
−100
−150
−200
−250
−300
−350
0
50
100
150
200
250
300
350
400

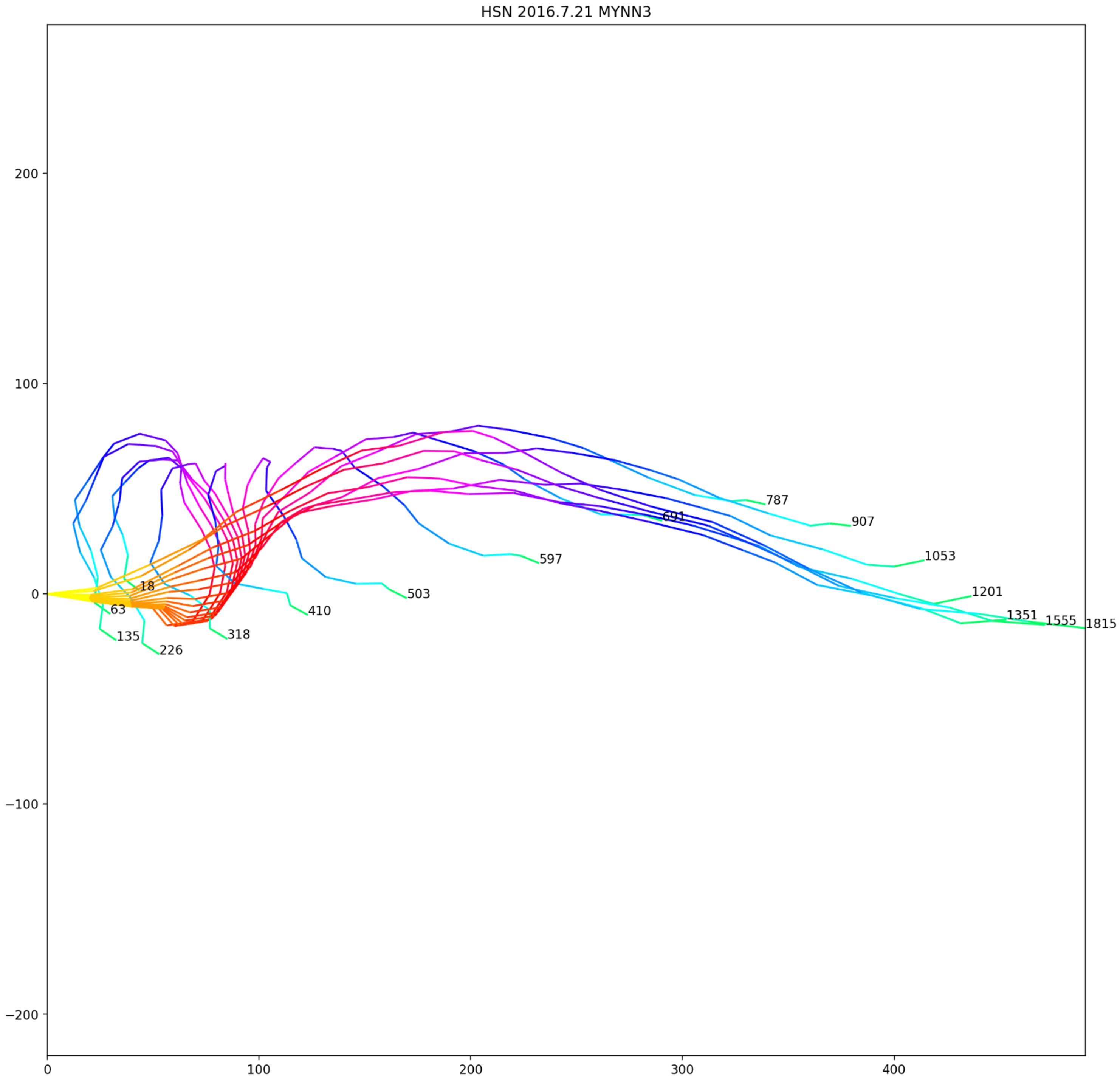

HSN 2016.7.21 YSU
50
0
−50
−100
−150
−200
−250
−300
0
50
100
150
200
250
300
350
400
18
63
136
228
320
413
507
602
697
793
914
1061
1210
1361
1566
1827



HSN 2016.7.21 ACM2
100
0
−100
−200
−300
0
100
200
300
400
1827
1566
1361
1210
1061
914
793
697
601
507
413
320
228
136
63
18


HSN 2016.7.21 MYJ
50
0
−50
−100
−150
−200
−250
−300
0
50
100
150
200
250
300
350
400
18
63
136
228
320
413
506
601
696
792
913
1059
1208
1359
1564
1825


HSN 2016.7.21 BouLac
50
0
−50
−100
−150
−200
−250
−300
0
50
100
150
200
250
300
350
400
1825
1564
1359
1208
1059
912
791
696
601
506
413
320
228
136
63
18



HSN 2016.7.21 MYNN3
200
100
0
−100
−200
0
100
200
300
400
18
63
135
226
318
410
503
597
691
787
907
1053
1201
1351
1555
1815

Summary

- Wind rotation is nearly ubiquitous during warm season
- Houston recirculation from sea breeze, DFW recirculation from remote low-level jet
- Modeling identifies age of ozone, using Nox-limited and VOC-limited production regimes
- WRF simulates recirculation and resulting pollutant buildup and transport on high-ozone days, but details are very sensitive to nudging and PBL scheme

Recommendations

- Utilize key meteorological predictors of stagnation/recirculation to predict ozone levels
  - Seasonal outlooks
  - Year-to-year variability
  - (Statistics/AI; reanalysis accuracy)
- Use age+source simulation technology
  - Improve process understanding of ozone
  - NOx/VOC limited on neighborhood/sub-daily scale
  - Case sensitivity to meteorology