



CITY OF SAN ANTONIO
METROPOLITAN HEALTH DISTRICT

Observational Analysis To Improve Understanding of Ozone Formation in San Antonio

Harvey E. Jeffries, PhD
Principal, OThree Chemistry, LLC

City Council B Session
October 17, 2018

Who is Jeffries ?

Professor Emeritus

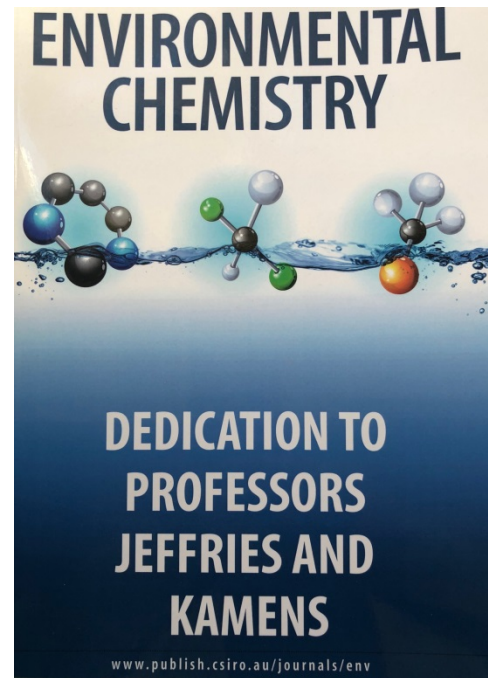
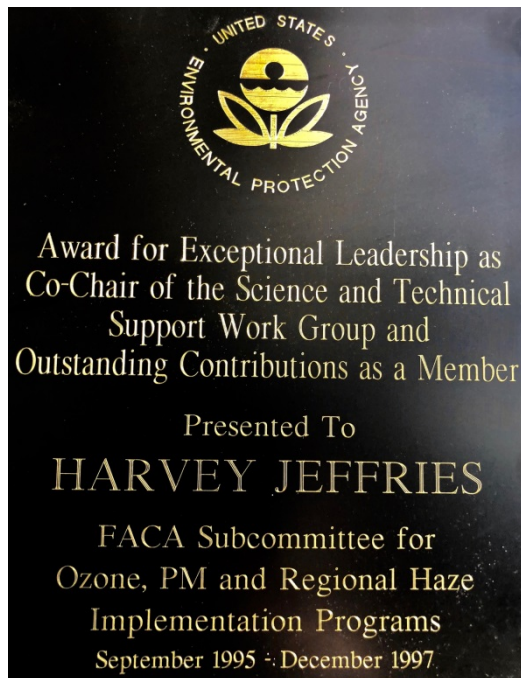
Atmospheric Chemistry
Department Environmental
Science and Engineering
Gillings School of Public Health
[University of North Carolina](#)
Chapel Hill, NC (44 years)

Science Advisor

Houston Eight-Hour Ozone
Coalition Stakeholders
National Urban Air Toxics Center
California Air Resources Board
US EPA Science Advisory Board
Advisory Council
California Air Resources Board
Reactivity Advisory

Service to

EPA's Office of Policy and Planning (OAQPS)
EPA's Office of Research and Development (ORD)



Observational Analysis

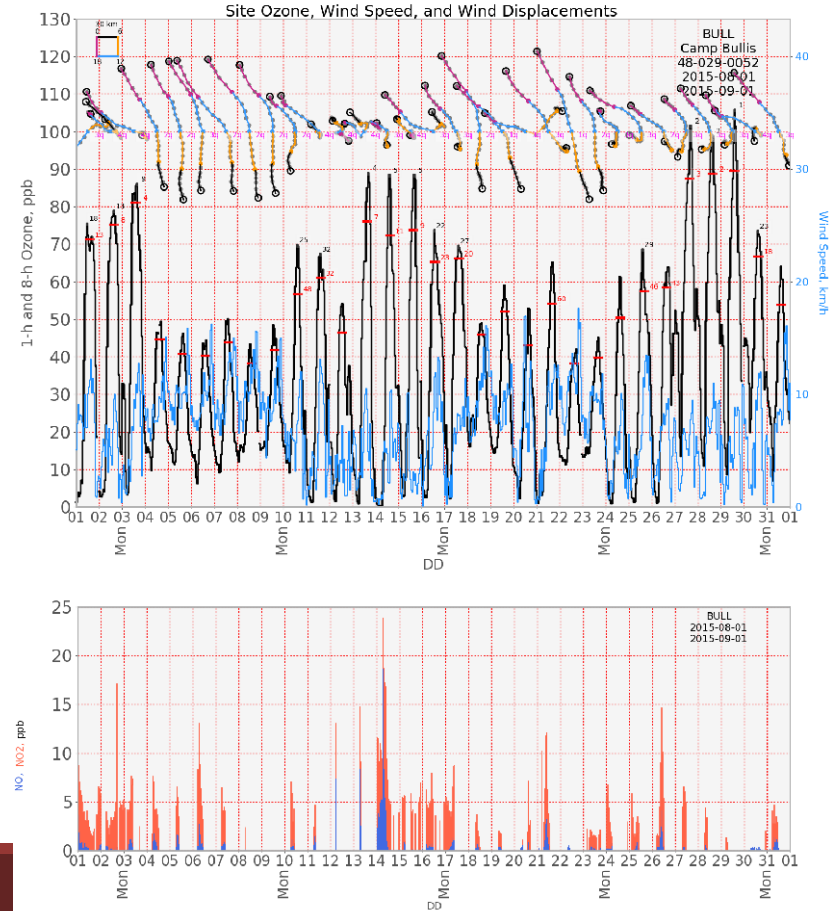
San Antonio Area 21 Monitor Sites
Data Available at Site = 1

Site	AIRS	TCEQ Name	O3	NOx	CO	AVOC	WD	SR	T	P	Rain	tot obs
MCRH	48-021-0684	CAPCOG McKinney Roughs C684	1	0	0	0	1	0	1	0	0	3
SANW	48-029-0032	San Antonio Northwest C23	1	1	0	0	1	0	1	0	0	4
SEAL	48-029-0051	San Antonio Seale A140	0	0	0	0	1	0	1	0	0	2
BULL	48-029-0052	Camp Bullis C58	1	1	0	0	1	1	1	0	0	5
PECV	48-029-0055	CPS Pecan Valley C678	1	1	1	0	1	0	1	0	0	5
CALA	48-029-0059	Calaveras Lake C59	1	1	0	0	1	0	1	0	0	4
ELMC	48-029-0501	Elm Creek Elementary C501	1	0	0	0	1	0	1	0	1	4
FORA	48-029-0502	Fair Oaks Ranch C502	1	0	0	0	1	0	1	0	1	4
HEMS	48-029-0622	Heritage Middle School C622	1	1	1	0	1	0	1	0	1	6
PALO	48-029-0676	Palo Alto C676	0	0	0	0	1	0	1	0	0	2
OLDH	48-029-0677	Old Highway 90 C677	0	0	0	0	1	0	1	0	0	2
I35N	48-029-1069	IH 35 C1069	0	1	0	0	1	0	1	0	0	3
BVES	48-091-0503	Bulverde Elementary C503	1	0	0	0	1	0	1	0	0	3
GARD	48-091-0505	City of Garden Ridge C505	1	0	0	0	0	0	0	0	0	1
NBAP	48-187-0504	New Braunfels Airport C504	1	0	0	0	0	0	0	0	0	1
SOLC	48-187-0506	Seguin Outdoor Learning Center C506	1	0	0	0	0	0	0	0	0	1
SMRS	48-209-1675	CAPCOG San Marcos Staples Road C1675	1	0	0	0	1	0	1	0	0	3
CCWT	48-355-0025	Corpus Christi West C4	1	0	0	0	1	1	1	0	0	4
CCTU	48-355-0026	Corpus Christi Tuloso C21	1	0	0	0	1	0	1	0	0	3
FLHB	48-493-1038	Floresville Hospital Blvd C1038	0	1	0	1	1	0	0	0	0	3
KARN	48-493-1070	Karnes County C1079	0	1	0	1	1	0	0	0	0	3
tot sites			15	8	2	2	18	2	16	0	3	92

- SANA has 21 air quality monitoring sites – only 3 are ‘regulatory’: BULL, SANW, CALA; others are ‘supporting’ (many have winds)
- These sites ‘report’ 1-H data to TCEQ for various species and meteorological parameters.

Observational Analysis

- My task was to turn these hourly data into “meaningful graphs and plots” and to contrast these among exceedances and non-exceedances for ozone and ‘to figure out’ why each occurred or not.
- Once these are understood, ‘causes’ can be changed so as to not exceed (if you have the right ‘**explanation**’).



What kinds of **Explanations** are there?

Quality of Explanation

Compelling

admits almost no other explanation

Preponderant

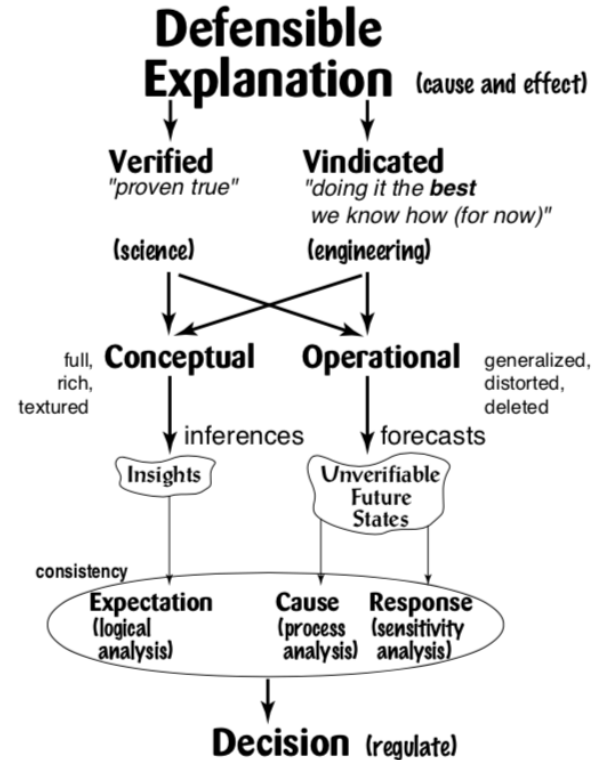
one explanation has more support than others (others also possible)

Permissive

nothing rules out explanation (others also possible)

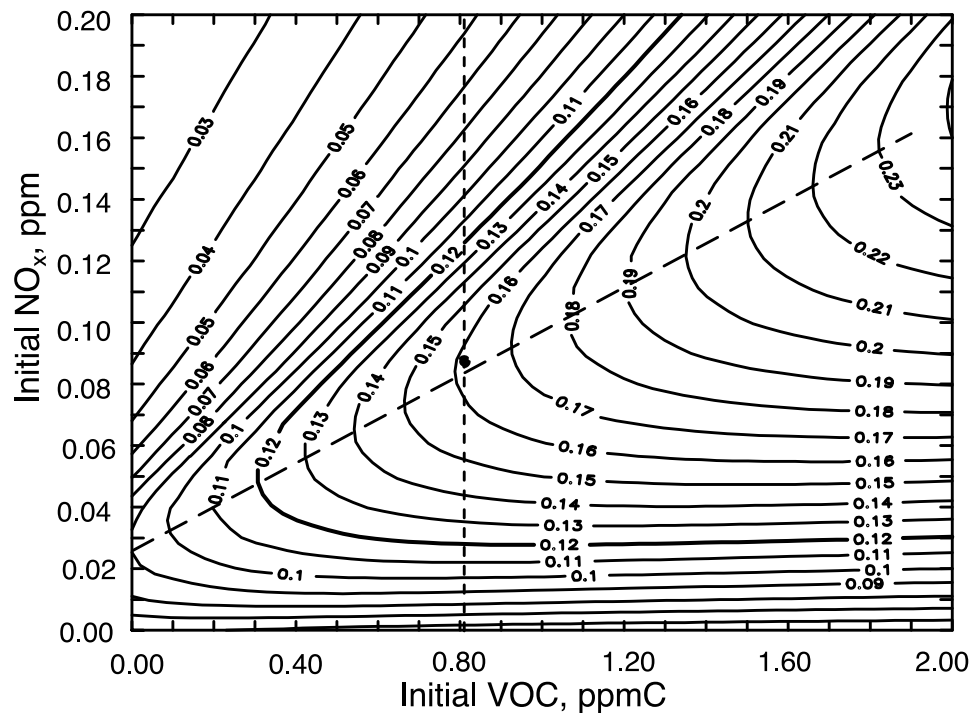
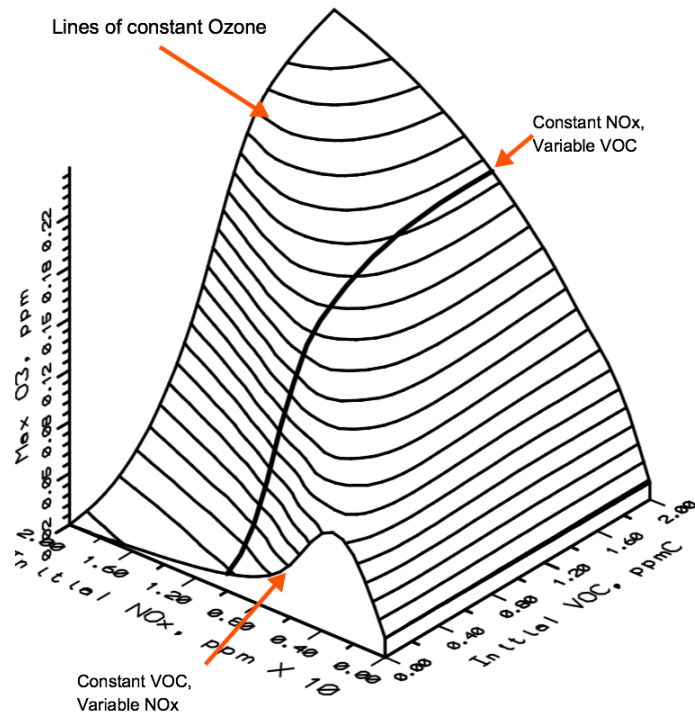
Missing

no explanation is available (all might be possible)



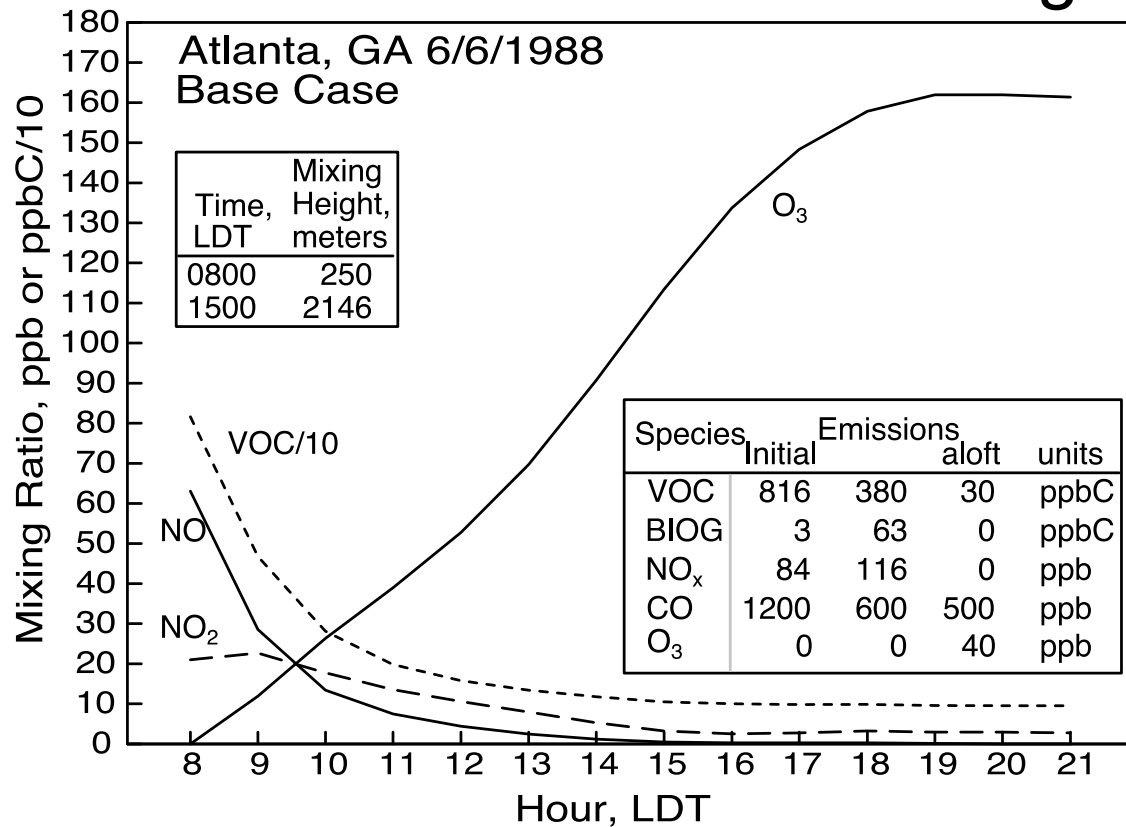
Harvey Jeffries, UNC

Ozone Not Emitted—Made in air from NO_x , VOCs at the earth's surface



Even While Being Diluted

NO_x & VOCs Can Make Increasing Ozone



In Urban Environments Many Physical and Chemical Processes Compete

- Emissions
- Dispersion
- Reactions
- Deposition

Wind observations are necessary for dispersion, dilution, transport

Chemical species observations are necessary for reactions, exposure, deposition

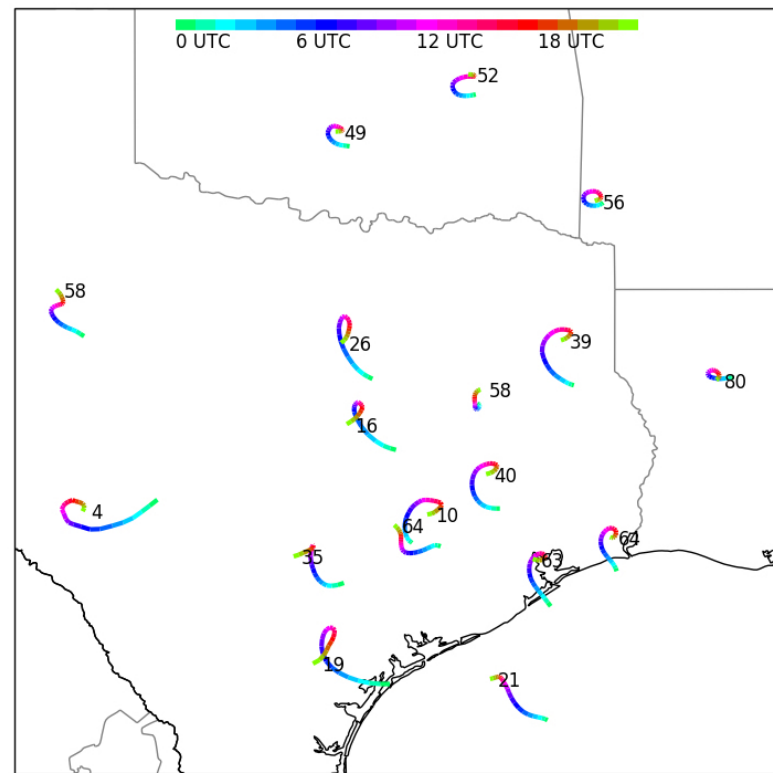
To Make Ozone in Texas Cities There Are
Necessary Wind Conditions
and
Sufficient Chemical Conditions

- **Necessary conditions** common to **all** San Antonio Ozone Exceedances are a daily **3Q** or **4Q** wind rotation (but see special **2Q** case below).
- Depending on the year, between 50 to 60 % of annual days at BULL site exhibit the necessary wind conditions, yet only 18 of these days exhibit an O₃ exceedance. *This is most likely caused by the sufficient chemical conditions not being achieved on all days.*
- **Sufficient chemical conditions** are related to NO_x and VOCs and radical sources like formaldehyde.

Texas Winds Rotate !

- Due to its 'unique' location on earth, 30° N latitude, interactions between the **Coriolis force** and the large scale **geostrophic (pressure gradient) forcing** results in 'rightward' rotation of wind direction during a day.
- At 30 N latitude, a full apparent rotation (a circle) requires **24** hours.
- (Courtesy of Prof. John Nielson-Gammon, Texas A&M University, 2018)(<https://www.youtube.com/watch?v=pBI-aKA-qAM>)

Rotating Winds in Upper Air Texas



Mean 500 mb 24-H Wind Flow to Statewide Sounders during TexAQS2 for May-October days with WS < 11 km/h and the number of days used is marked.

Byun's full formulation of atmospheric surface flow is

Gutman and Berkofsky (1985); Byun and Arya (1990) →

$$\frac{\partial \mathbf{V}_m}{\partial t} = \underbrace{-\mathbf{ADV}(\mathbf{V}_m)}_{[1]} - \underbrace{f\mathbf{k} \times (\mathbf{V}_m - \mathbf{V}_{Gm})}_{[2]} - \underbrace{\left[g' \nabla \cdot \boldsymbol{\eta} - \left(\frac{gh}{2\Theta_0} \right) \nabla \cdot \boldsymbol{\Theta}_m \right]}_{[3]} - \underbrace{\frac{C_d}{h} |\mathbf{V}_m| \mathbf{V}_m}_{[4]} \quad (1)$$

[1] Local tendency

[2] Advection

[3] Coriolis forcing

[4] Large-scale pressure gradient (or geostrophic) forcing

[5] Local thermal forcing

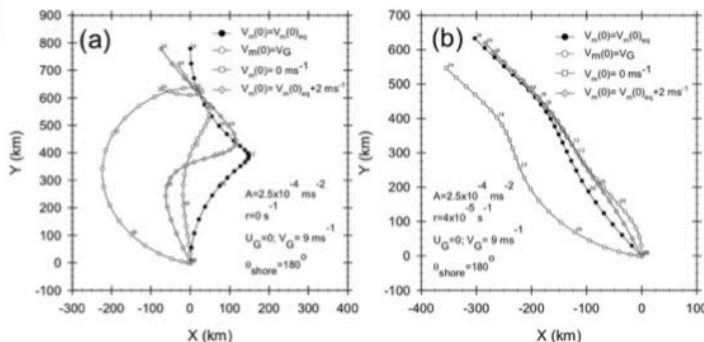
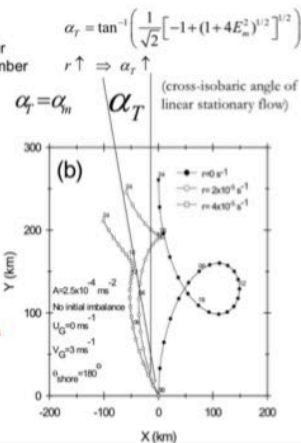
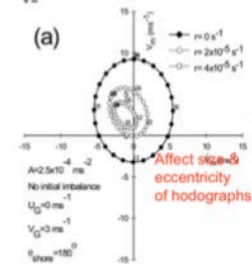
[6] Turbulent drag – Quadratic friction (no entrainment assumption)

Role of friction

Byun and Arya (1990)

Mixed Layer
Ekman Number

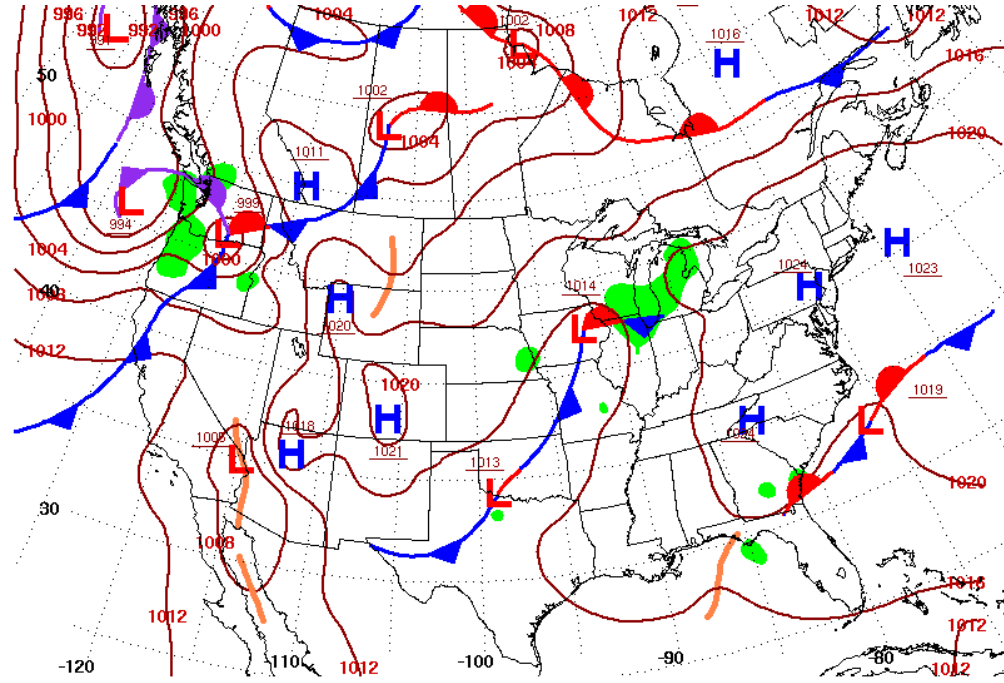
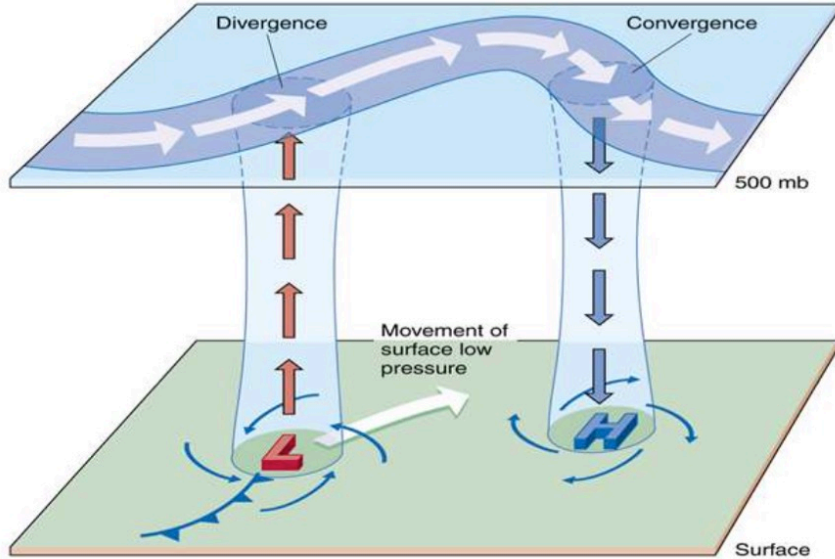
$$E_m \equiv C_d |\mathbf{V}_{Gm}| / fh$$
$$r = \frac{f}{\sqrt{2}} \left[-1 + (1 + 4E_m^2)^{1/2} \right]^{1/2}$$



- 1) The amplitude of the initial imbalance affects the trajectory shapes greatly from the self-intersecting shape, cusp shape, to the smooth curve, and the frictional effect reduces the differences in the trajectory patterns.
- 2) The equilibrium orbits are similar to each other except for the zero wind case, but the time to reach the equilibrium may change depending on the initial amplitude

Daewon Byun
(U of H)
solved this
problem in
2005

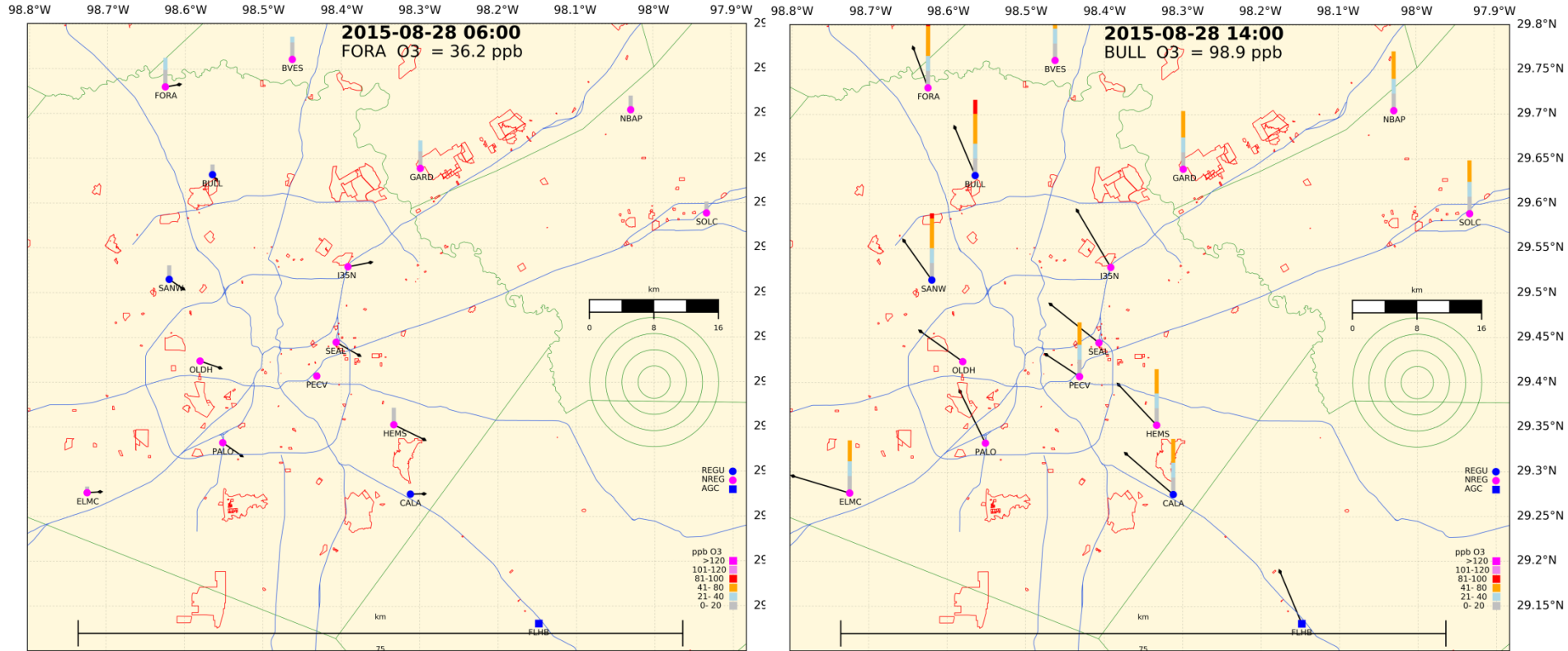
Large-scale Pressure Gradient (geostrophic forcing)



2015-08-29 06 CST

Surface Weather Map at 7:00 A.M. E.S.T.

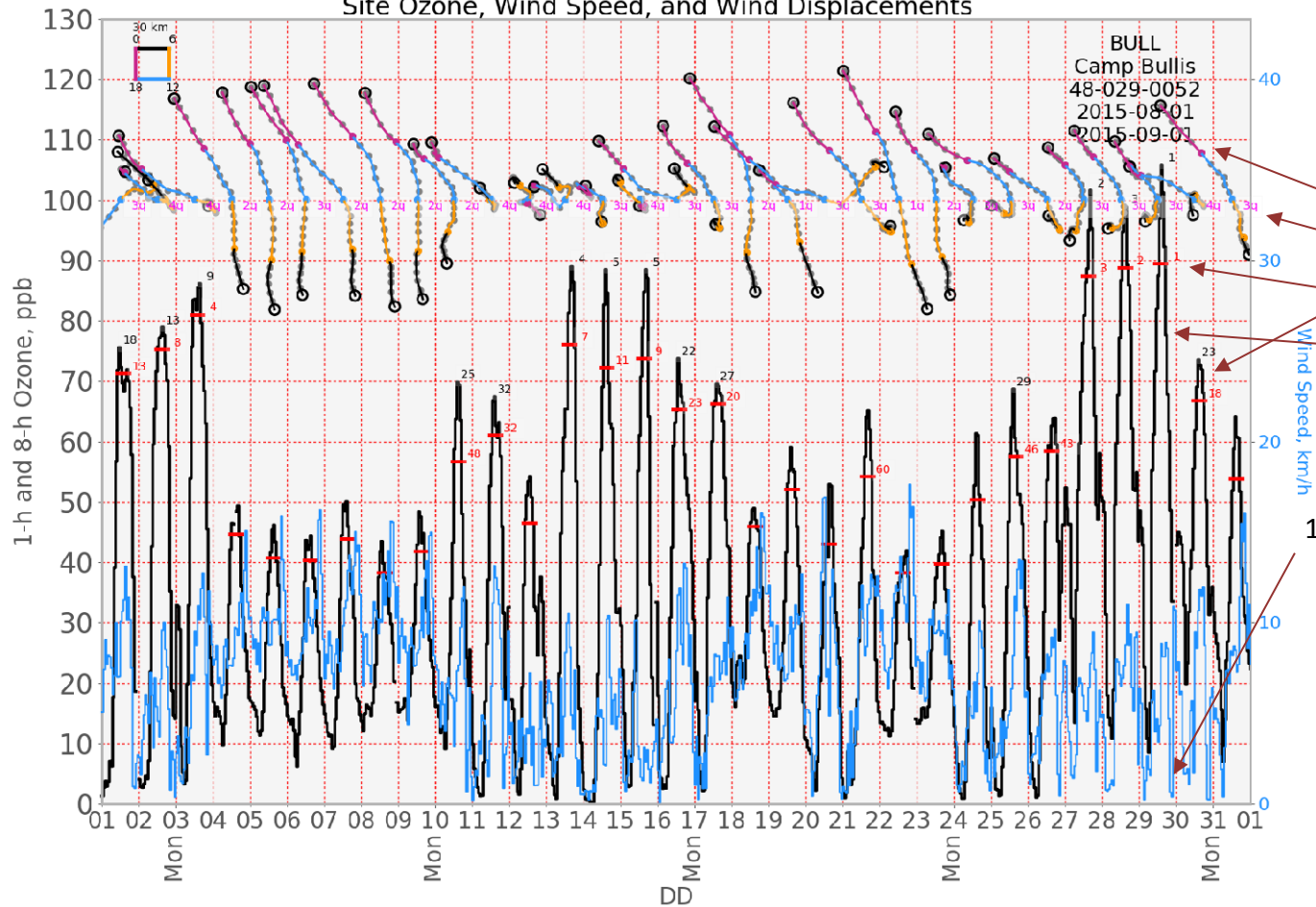
San Antonio Winds Rotate On High Ozone Days



Hourly Observations and Ozone Exceedances

- How often are there O_3 exceedances?
- Other than nQ winds characteristics are there other characteristics?
 - What is the 'range' of daily 1-H O_3 ? 'Transported O_3 '? 'NO Titrated O_3 '?
- Which direction does the NO_x and VOC come from? From how far?

Site Ozone, Wind Speed, and Wind Displacements



August 01, 2015
September 01, 2015

Displacement Wind Trajectory
nq = Number Wind Quads/day

8-H ozone, rank 1, 20

1-H ozone, rank 1

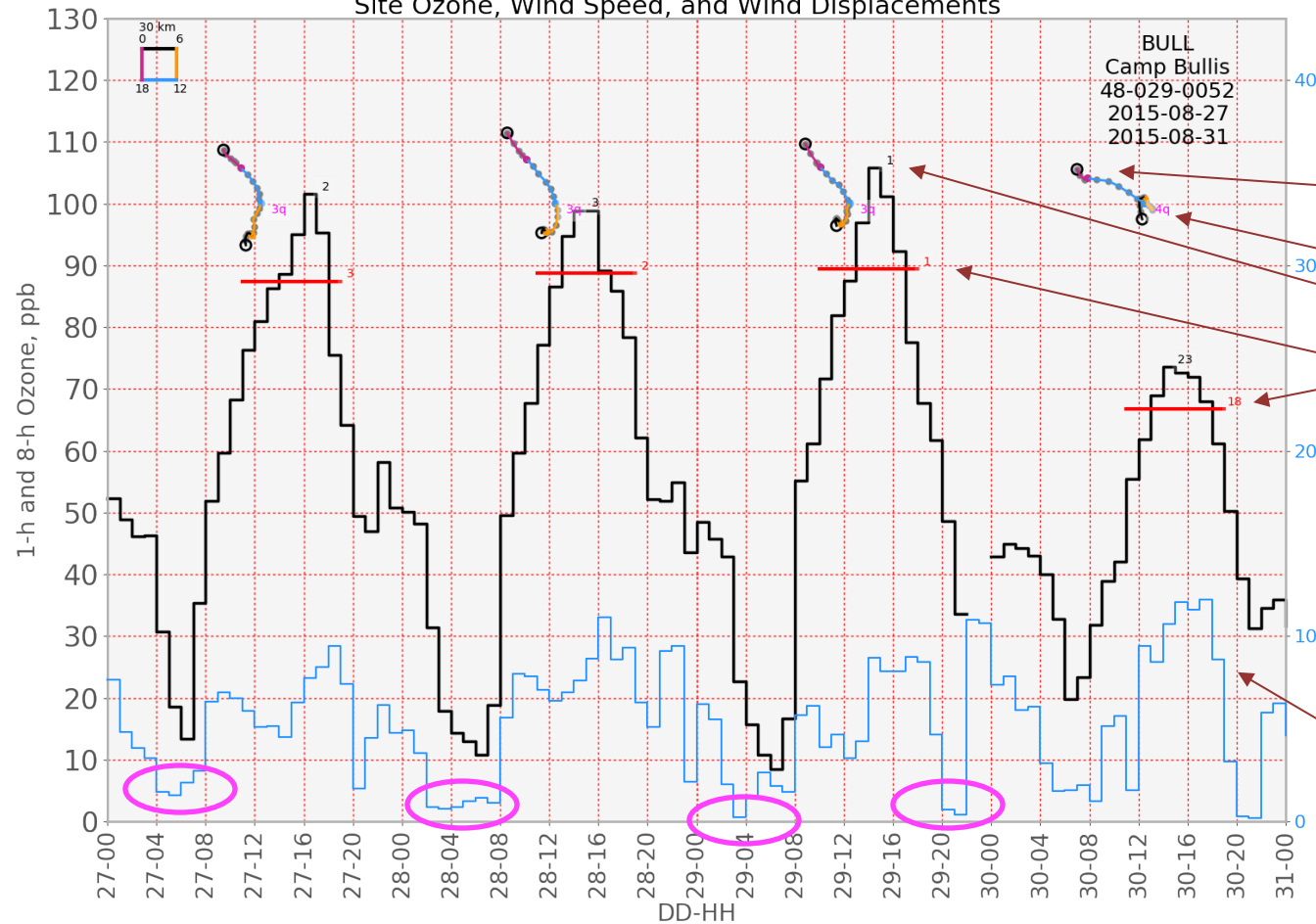
Wind
Displacement
Distance Scale

1-H wind speed

AUGUST 2015

SUN	MON	TUE	WED	THU	FRI	SAT
						1 213
2 214	3 215	4 216	5 217	6 218	7 219	8 220
9 221	10 222	11 223	12 224	13 225	14 226	15 227
16 228	17 229	18 230	19 231	20 232	21 233	22 234
23 235	24 236	25 237	26 238	27 239	28 240	29 241
30 242	31 243					

Site Ozone, Wind Speed, and Wind Displacements



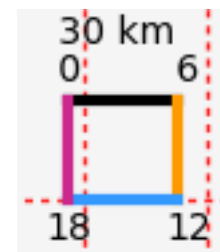
August 27, 2015
August 31, 2015

Displacement Wind Trajectory

nq = Number Wind Quads/day

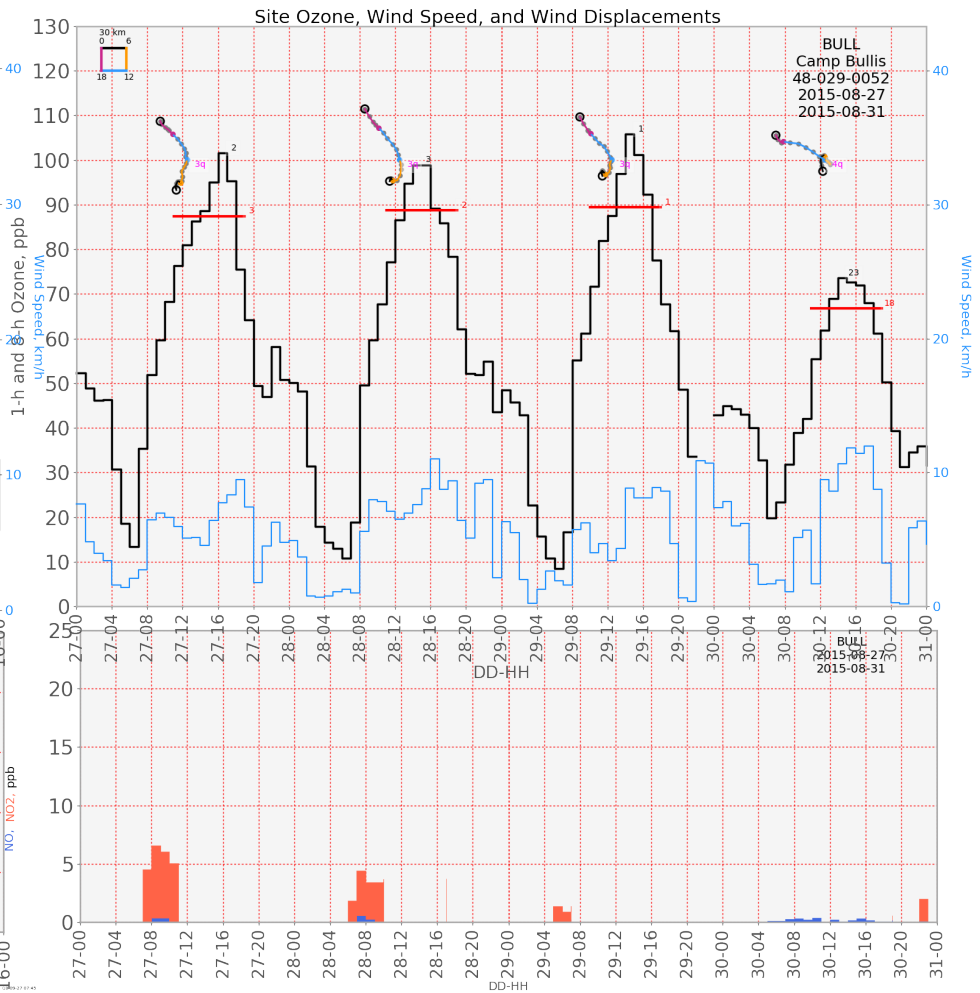
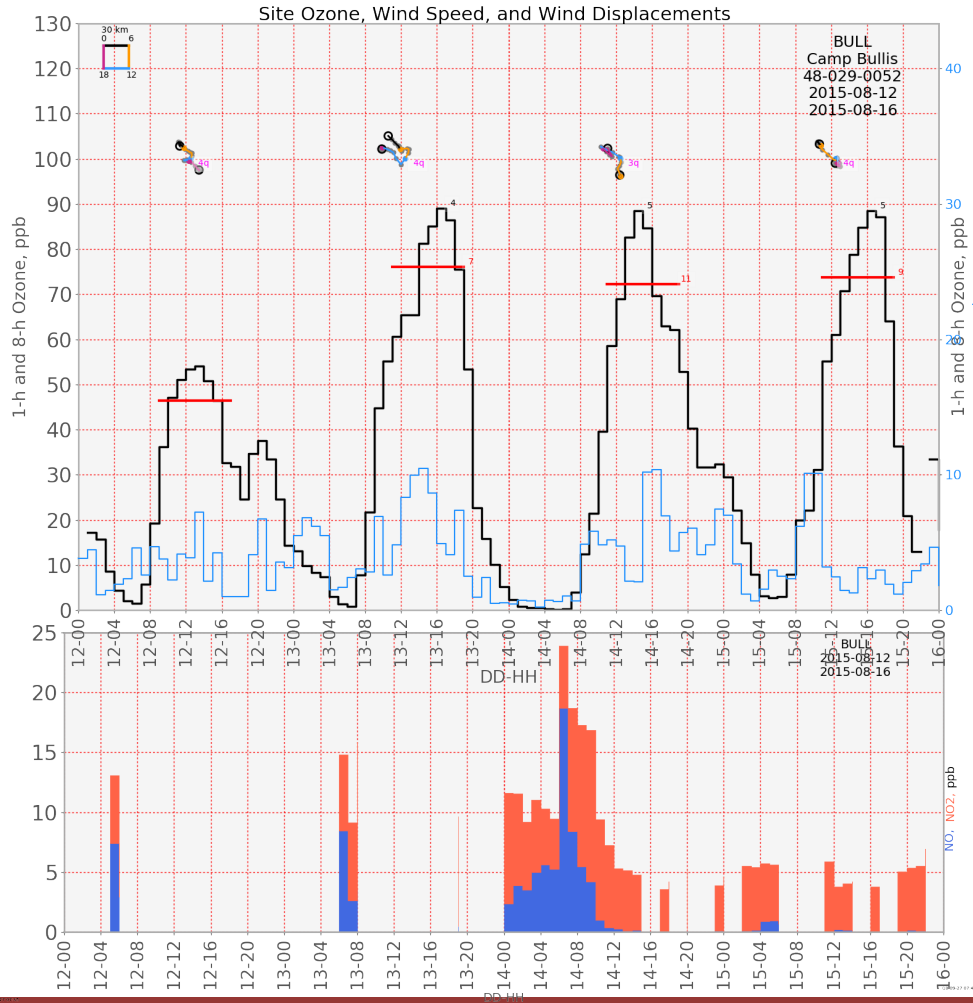
1-H ozone, rank 1

8-H ozone, rank 1, 18



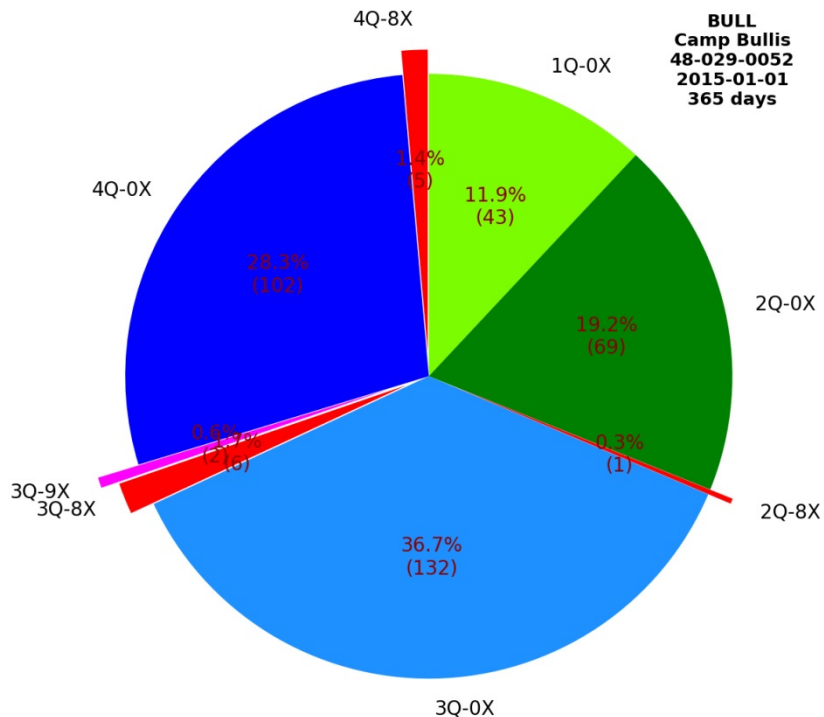
Wind Displacement Distance Scale

1-H wind speed



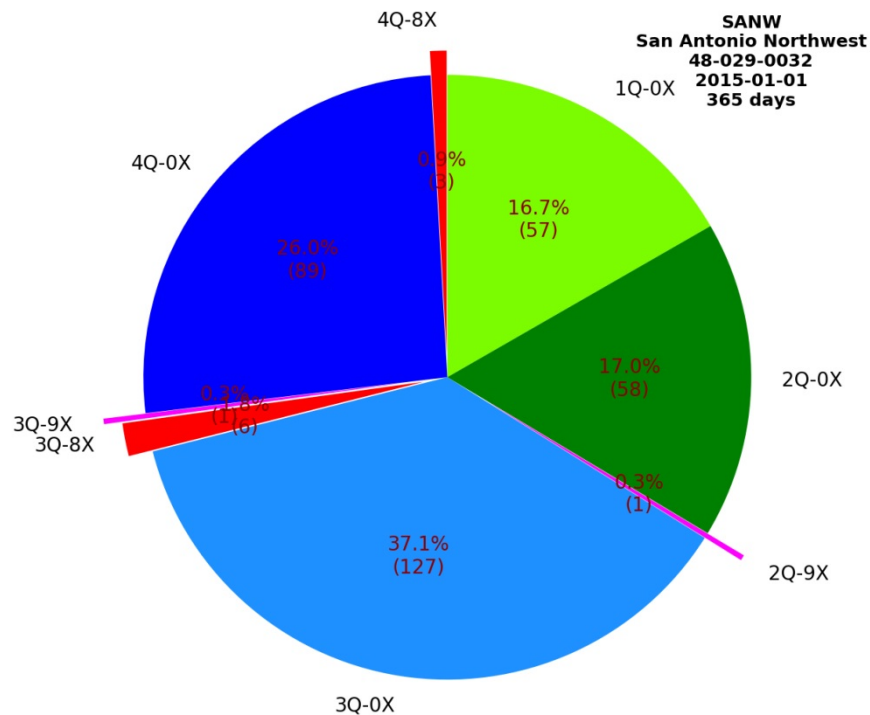
2015 Wind Quadrants and O₃ Exceedances

Daily Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)



1X days are rank 1-15 annual days with O₃1H ≥ 100 ppb
 8X days are rank 1-20 annual days with O₃8H ≥ 70 ppb
 9X days have both 1X and 8X exceedances

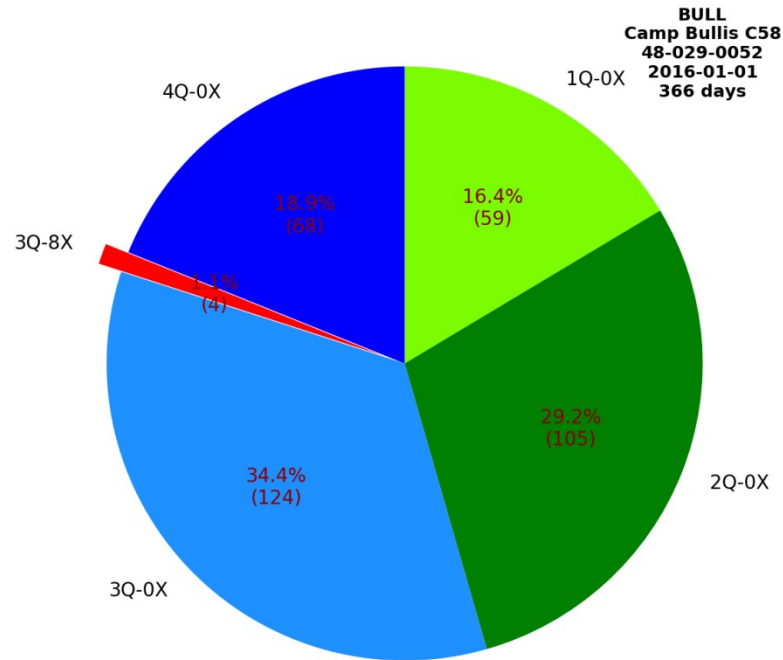
Daily Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)



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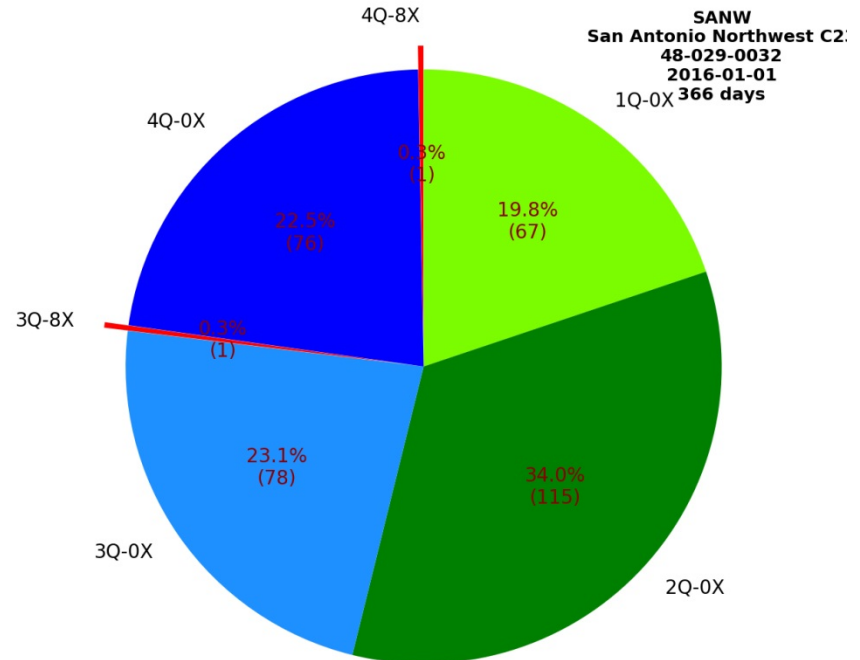
2016 Wind Quadrants and O₃ Exceedances

Daily Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)



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 8X days are rank 1-20 annual days with O₃8H >= 70 ppb
 9X days have both 1X and 8X exceedances

Daily Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)

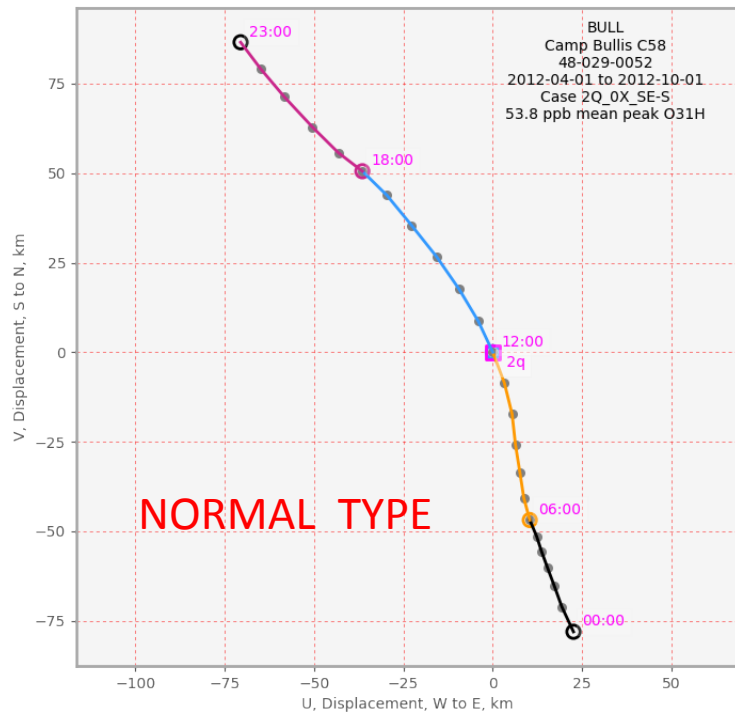


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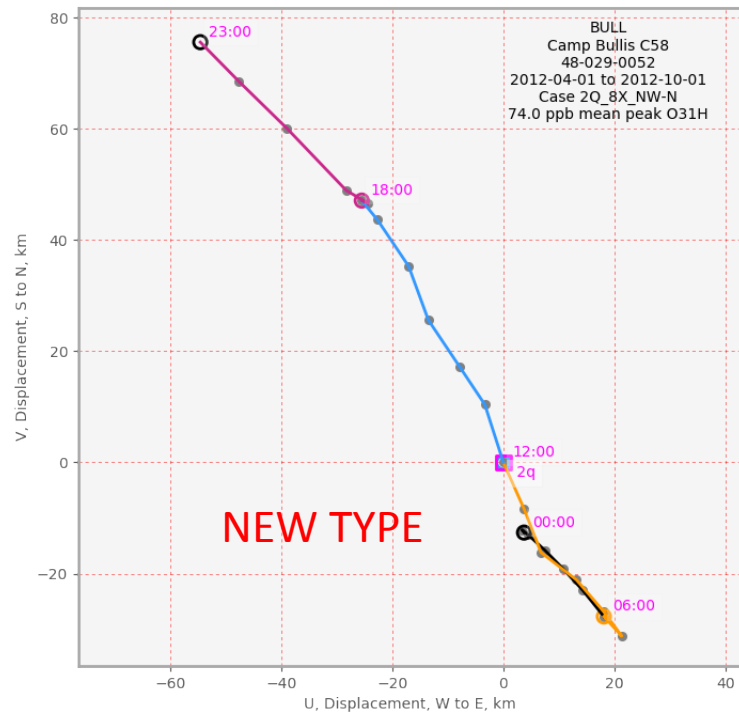
2015 2Q 0X and 2Q 8X Displacement Trajectories

New Type Exceedance Wind Flow seen in San Antonio (rare)

Mean U and V Hourly Displacement From Noon At Site (26 Days)



Mean U and V Hourly Displacement From Noon At Site (1 Days)

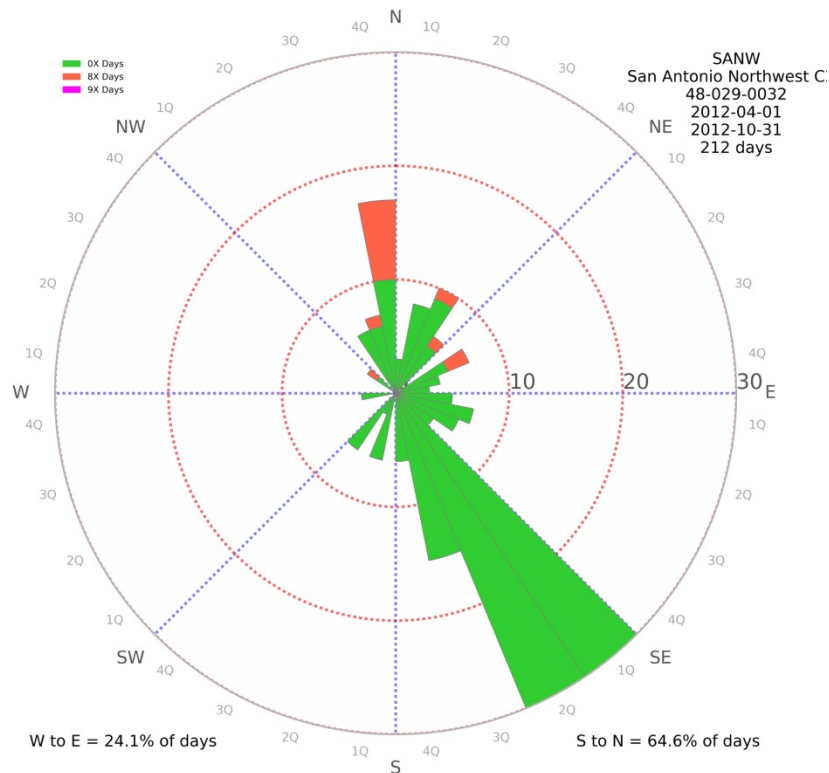


San Antonio, Houston, El Paso Have Similar Wind Distributions 2012, 2015, 2016

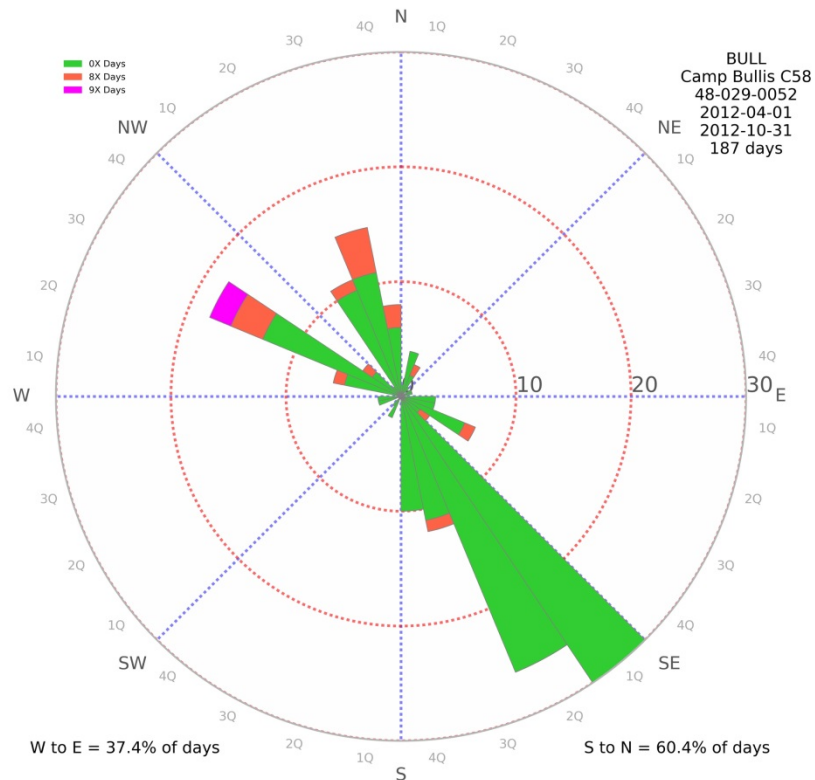
- As expected, BULL and SANW had similar nQ distributions in each year
- As expected, San Antonio, Houston, and El Paso had similar nQ distributions each year.
- Distribution among $1Q$, $2Q$, $3Q$, $4Q$ each year tends to change bi-annually due to the El Niña/La Niña global cycle that changes large scale flows across the southern US.

2012 Morning Wind Octet, Quads, O₃ Exceedances

Days by Morning Winds, Daily Wind Quads, and Ozone Exceedances

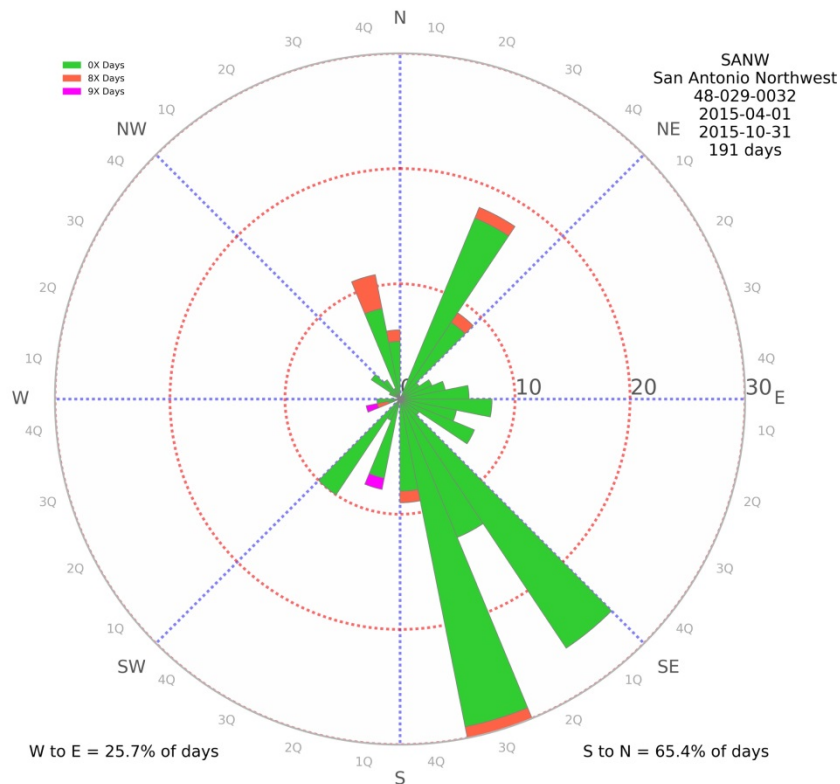


Days by Morning Winds, Daily Wind Quads, and Ozone Exceedances

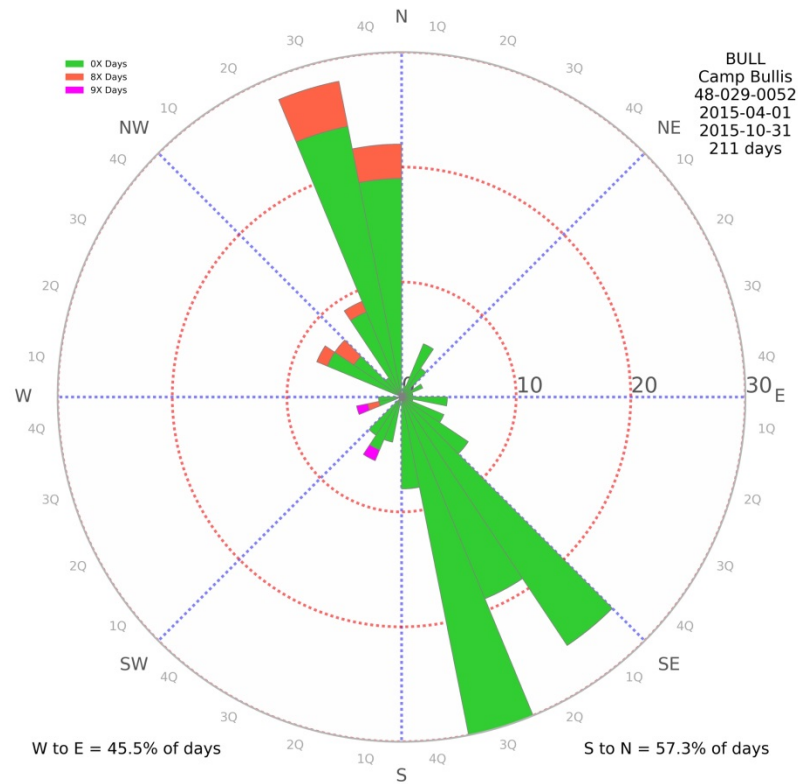


2015 Morning Wind Octet, Quads, O₃ Exceedances

Days by Morning Winds, Daily Wind Quads, and Ozone Exceedances

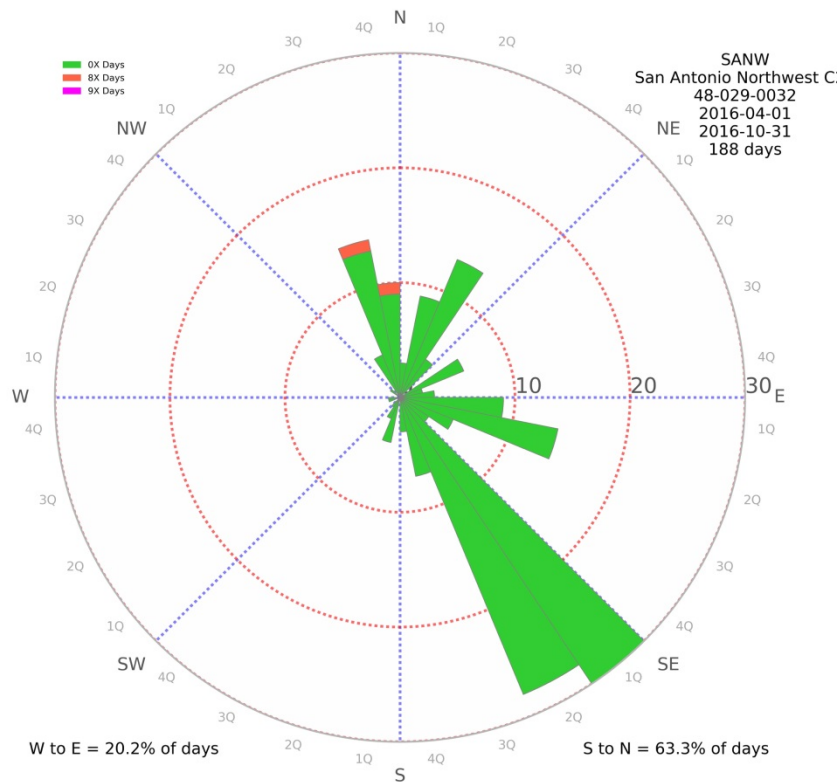


Days by Morning Winds, Daily Wind Quads, and Ozone Exceedances

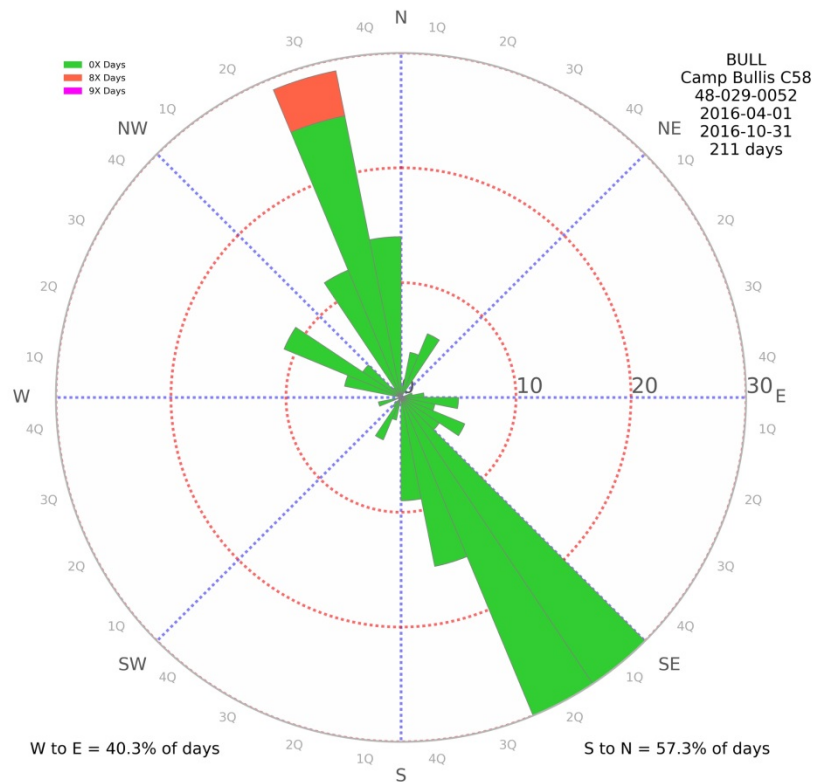


2016 Morning Wind Octet, Quads, O₃ Exceedances

Days by Morning Winds, Daily Wind Quads, and Ozone Exceedances



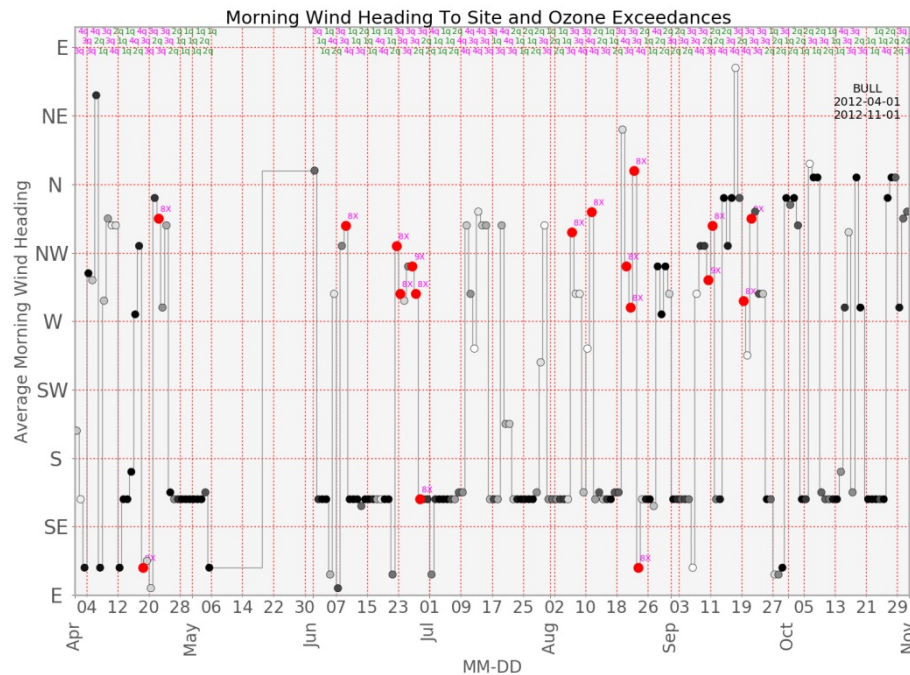
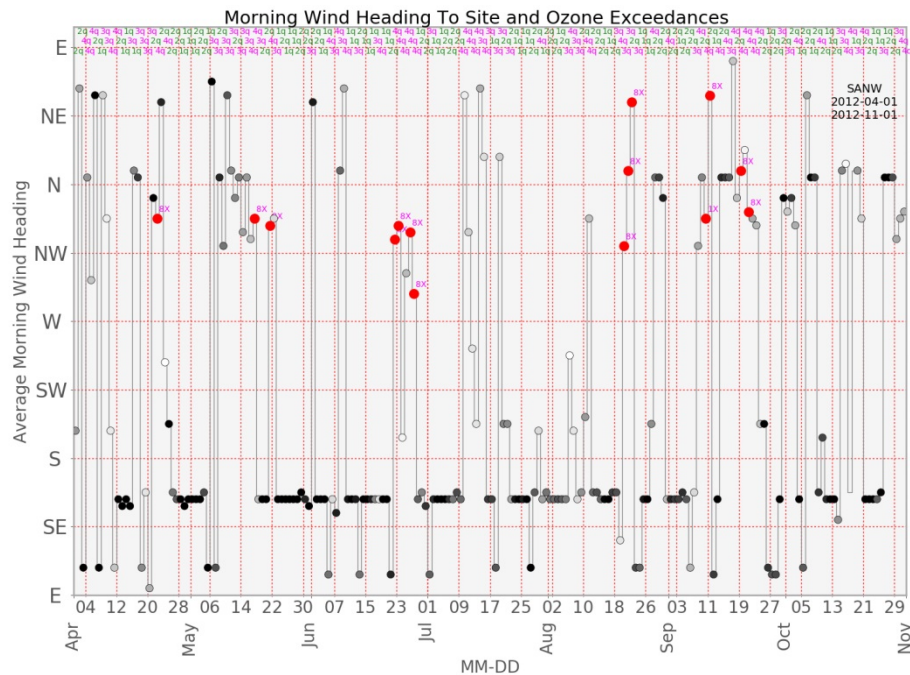
Days by Morning Winds, Daily Wind Quads, and Ozone Exceedances



2012 Morning Wind Octet Timeseries

Dot Color = Wind Speed Gray Scale
Black > 40 km/h White < 4 km/h

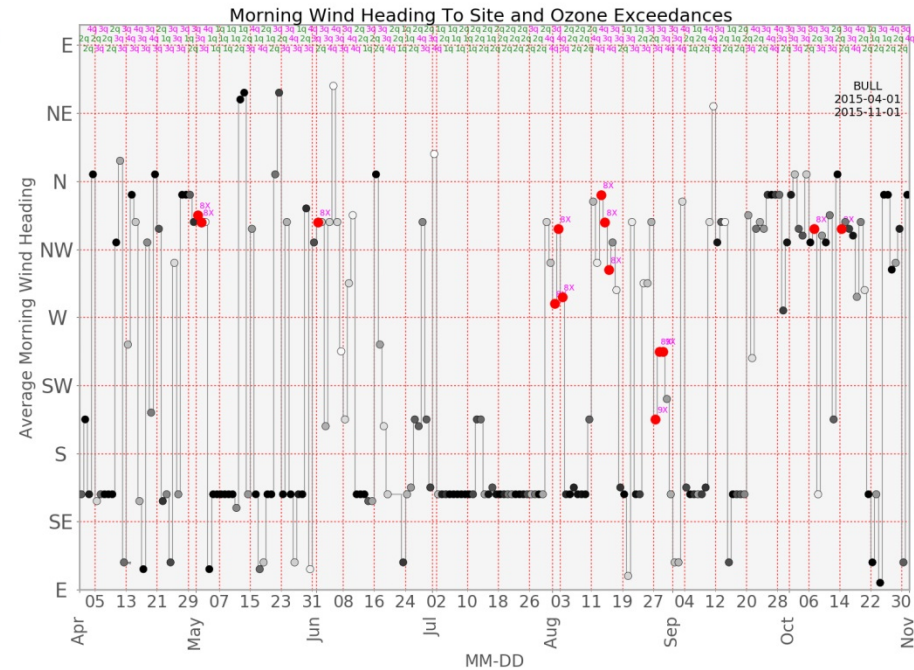
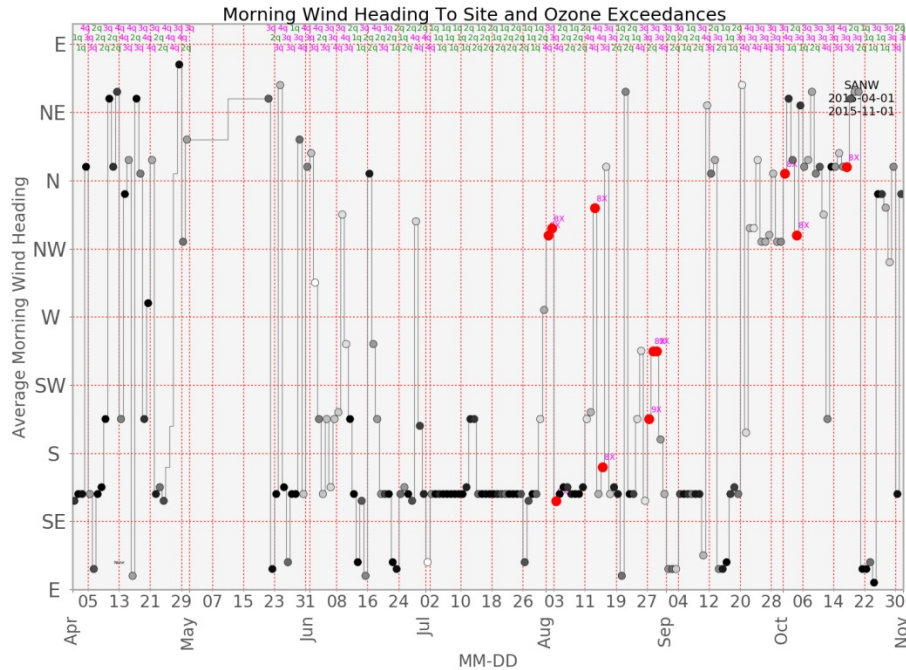
Red Dot Color = O₃ exceedance 8X or 9X



2015 Morning Wind Octet Timeseries

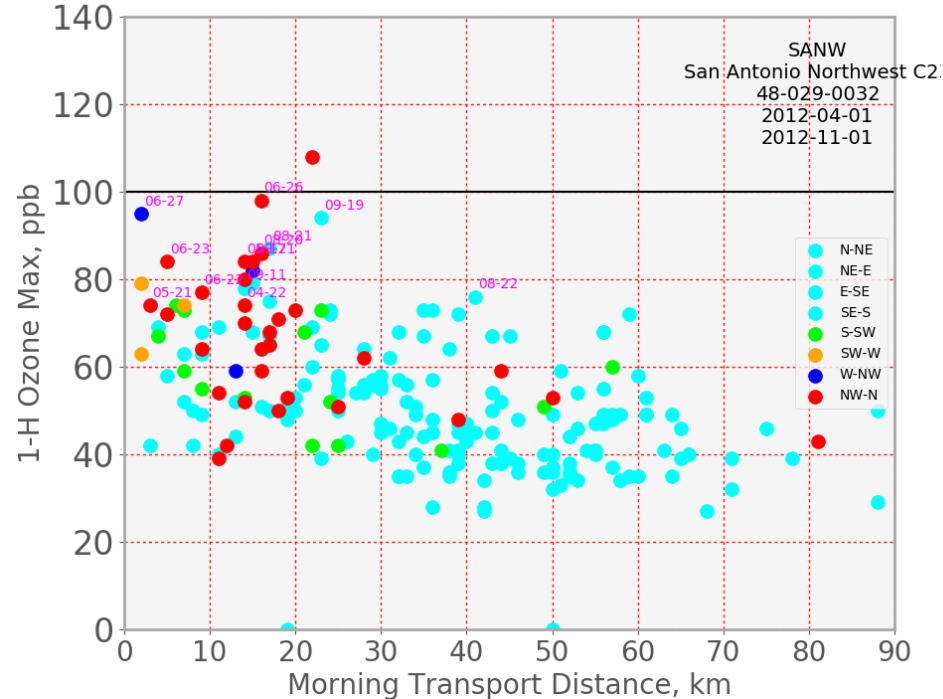
Dot Color = Wind Speed Gray Scale
Black > 40 km/h White < 4 km/h

Red Dot Color = O₃ exceedance 8X or 9X

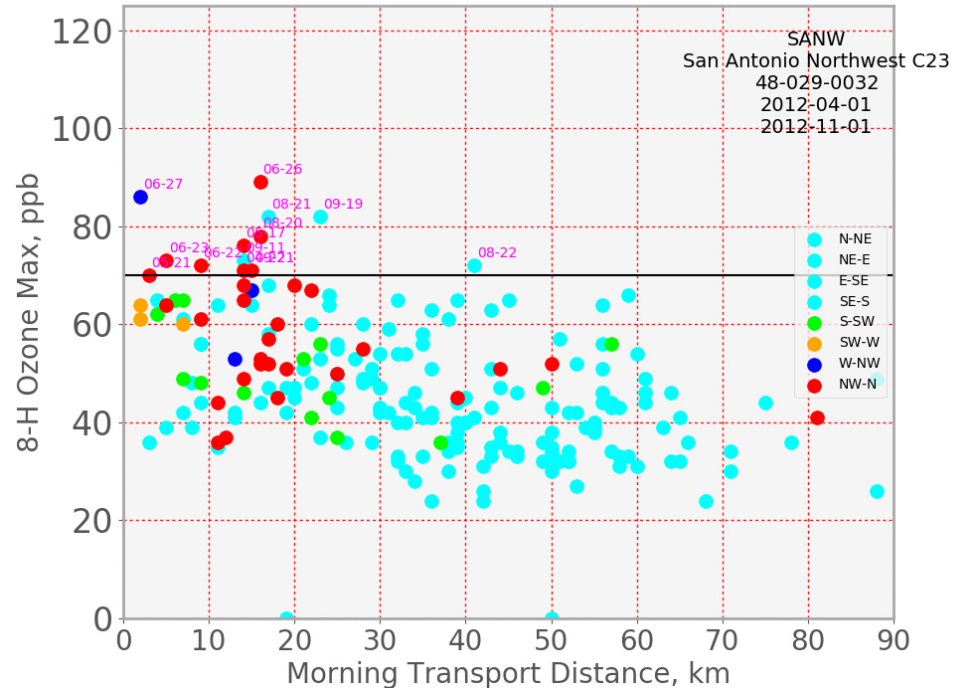


2012 SANW O₃ (1H), (8H) vs 00-06 HH Transport Distance

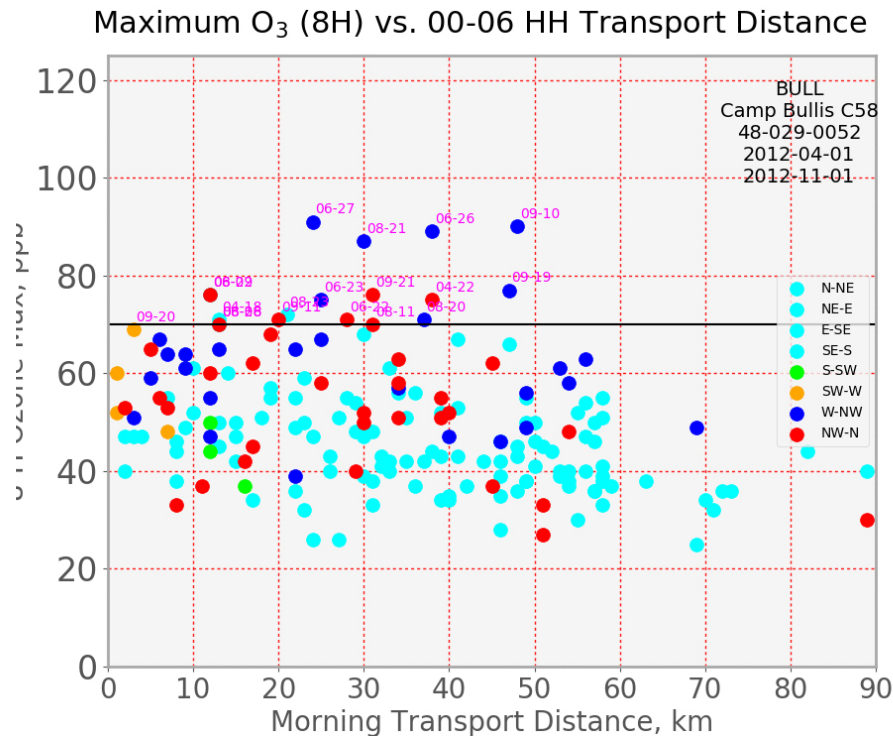
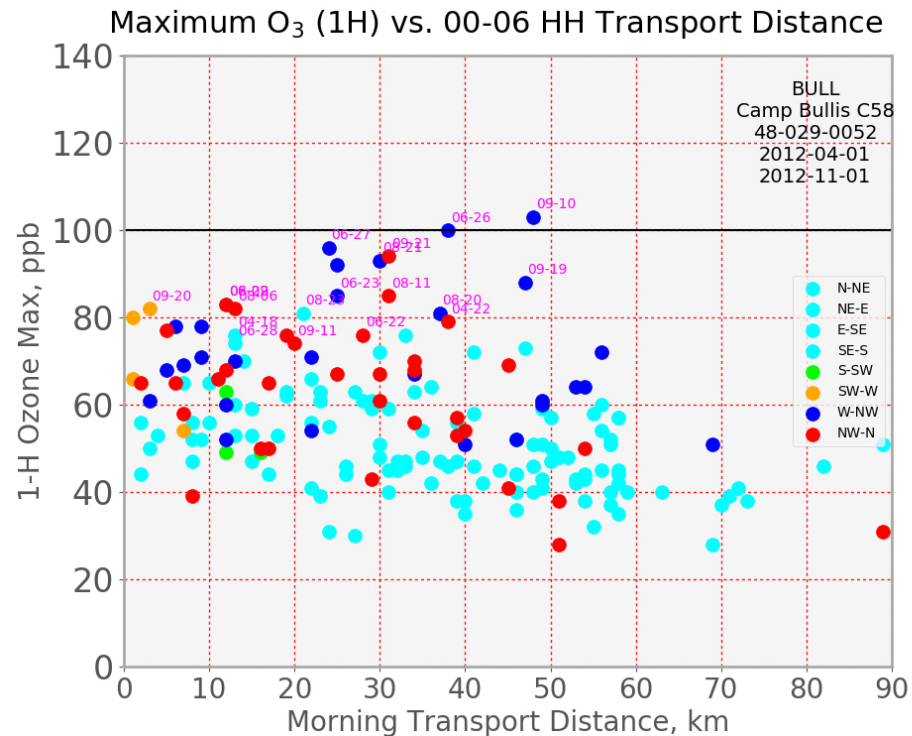
Maximum O₃ (1H) vs. 00-06 HH Transport Distance



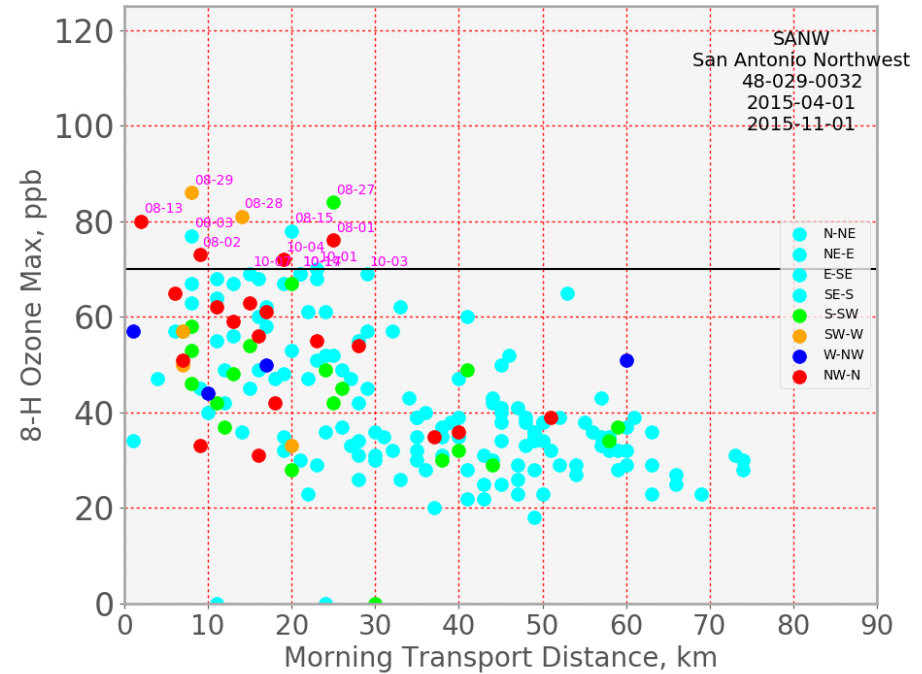
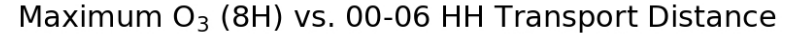
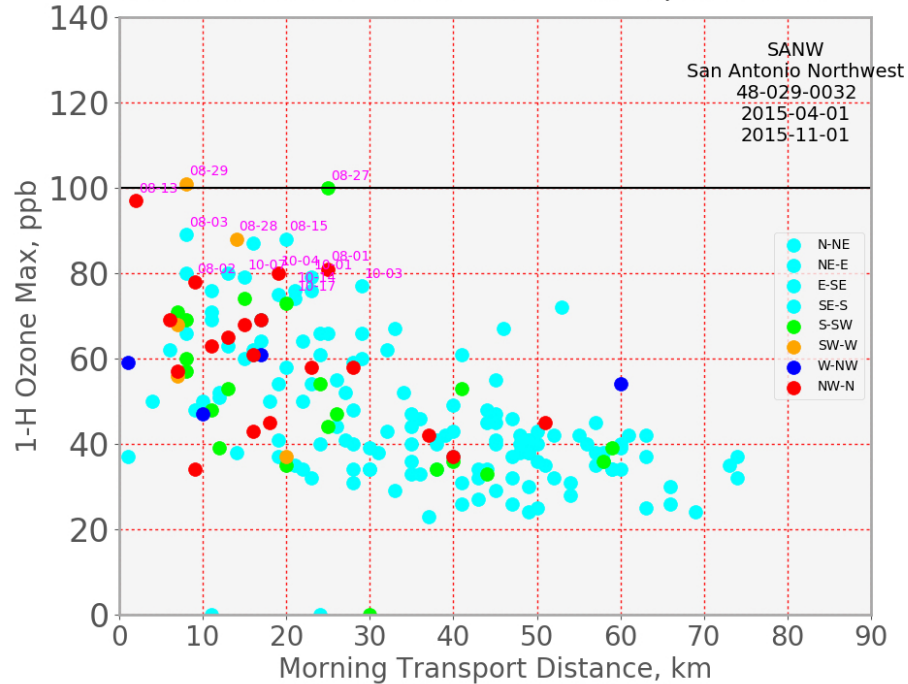
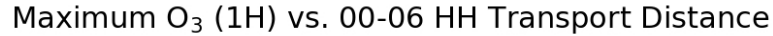
Maximum O₃ (8H) vs. 00-06 HH Transport Distance



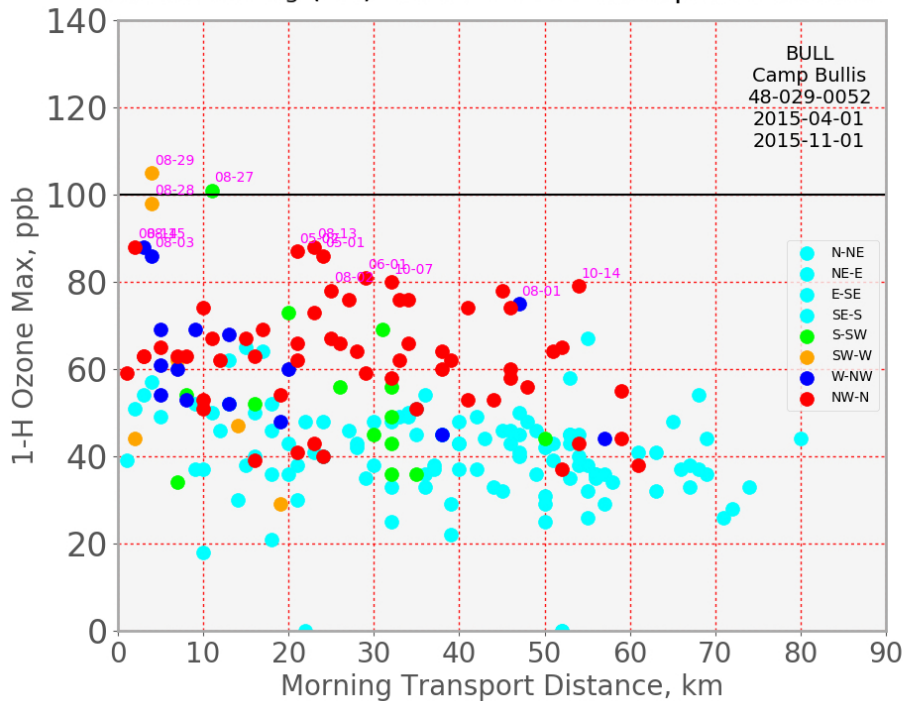
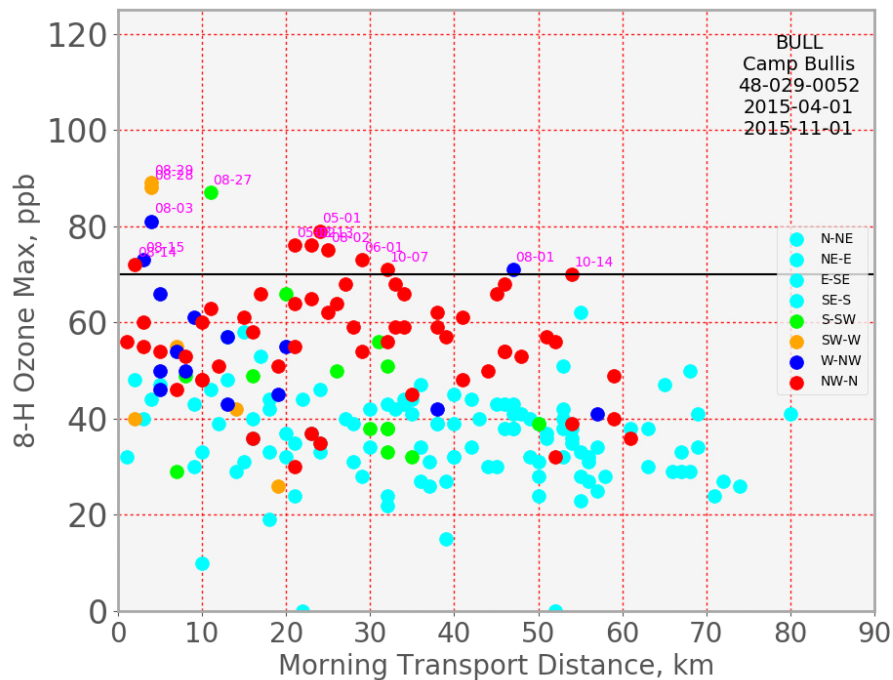
2012 BULL O₃ (1H), (8H) vs 00-06 HH Transport Distance



2015 SANW O₃ (1H), (8H) vs 00-06 HH Transport Distance



2015 BULL O₃ (1H), (8H) vs 00-06 HH Transport Distance

Maximum O₃ (1H) vs. 00-06 HH Transport DistanceMaximum O₃ (8H) vs. 00-06 HH Transport Distance

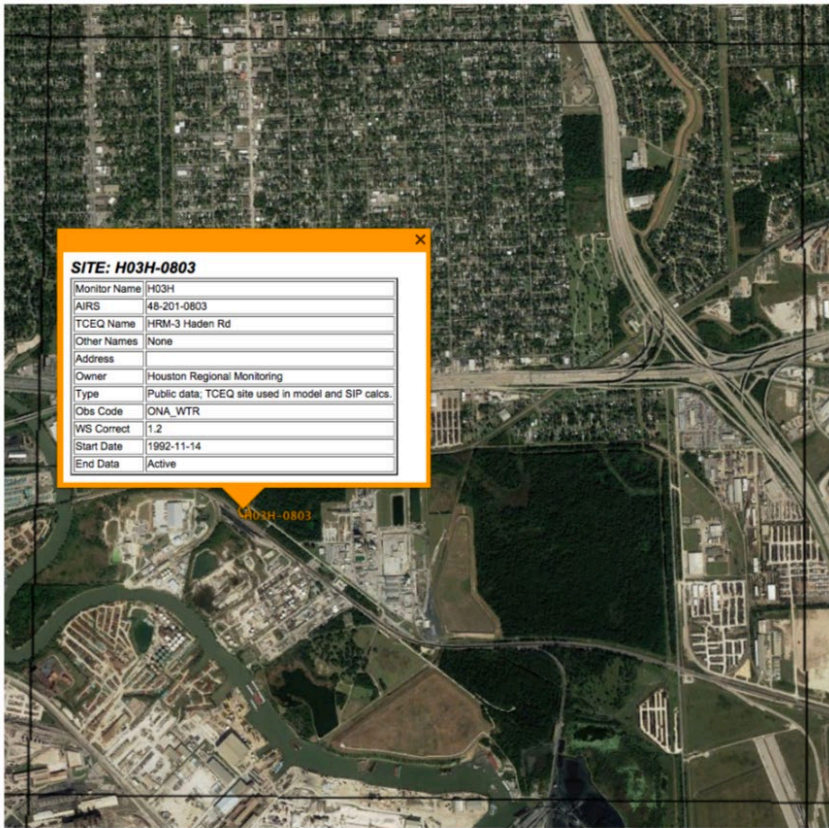
TCEQ's CAMx Model 152-Day Scenario for 2012

Used by Alamo Area Council of Governments for San Antonio Area
and Alpine Geophysics for Houston 8-Hour Coalition

- The TCEQ 2012 152-day CAMx Model simulation with nested grids is likely to be used by TCEQ for estimating 2020 8-H ozone control requirements. The highest resolution grid is 4-km cells, extending from west of San Antonio to east of Houston.
- Both AACOG and AG have re-run the full scenario and have model-derived data. Jeffries asked AACOG for layer-one, 4-km grid model selected species predictions for 152 days. They were not able to supply these until the last month of OThree's Contract, too late for Jeffries to use them for analysis. AG was able to supply all Houston monitors species predictions in August 2018.
- Here, I have used monitor site observations from 2012 Houston and the AG extracted layer one for grids the 152 day CAMx predicted species. For here, for now, I am focused only on ozone, but the same suite of graphs and plots for ambient data will be applied to the model data.

Houston's H03H Monitor in TCEQ's CAMx 4-km Grid

Data extracted from Alpine Geophysics Run of TCEQ's 2012 Model



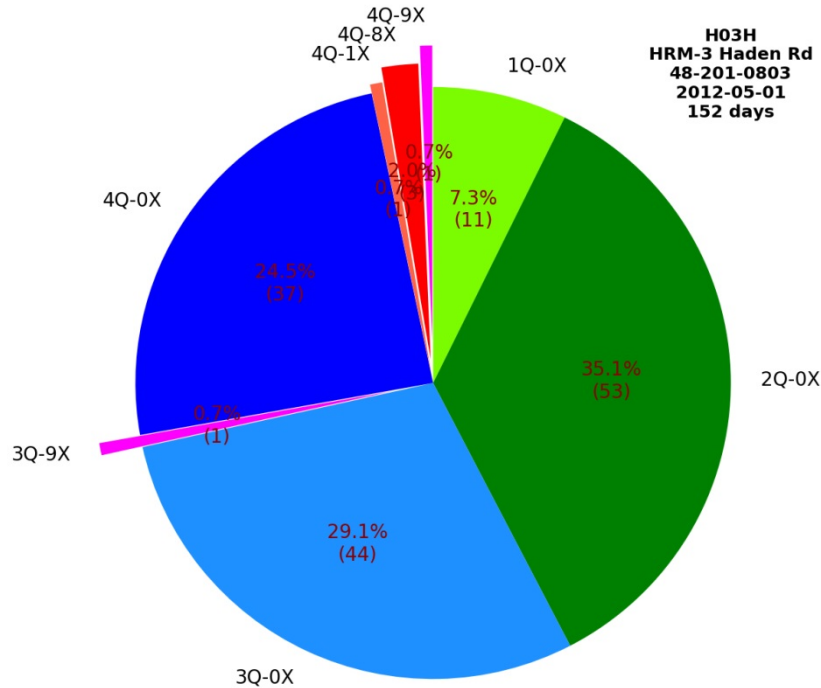
Single 4-kilometer CAMx Model Grid (black lines) containing Houston H03H TCEQ Monitor

Model predicts one set of mixing ratios for whole cell and layer.

Model predicts U- and V- components of the wind at left edge and bottom edge and layer.

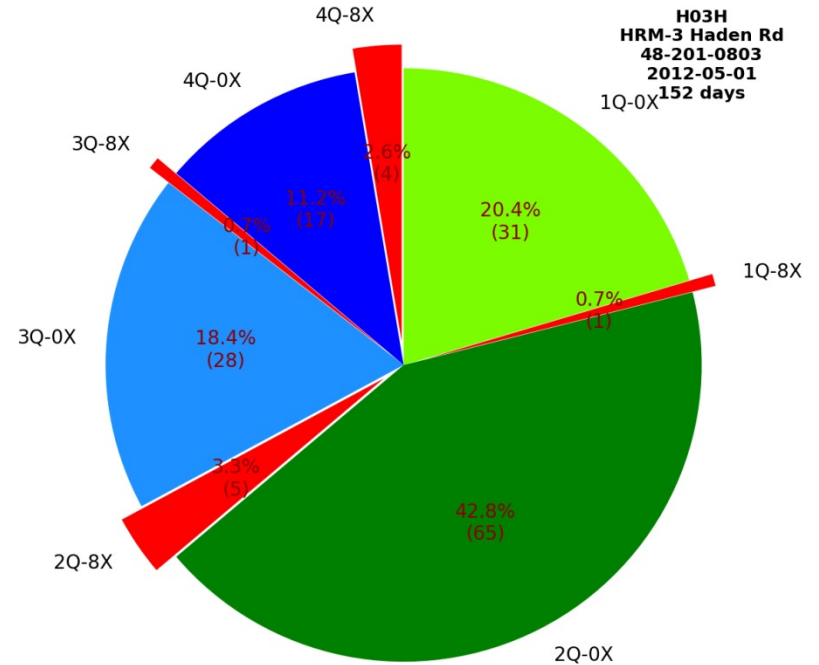
2012 H03H Observed and Model Predicted Wind Quadrants and O₃ Exceedances

Observed Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)



1X days are rank 1-15 annual days with O31H >= 100 ppb
8X days are rank 1-20 annual days with O38H >= 70 ppb
9X days have both 1X and 8X exceedances

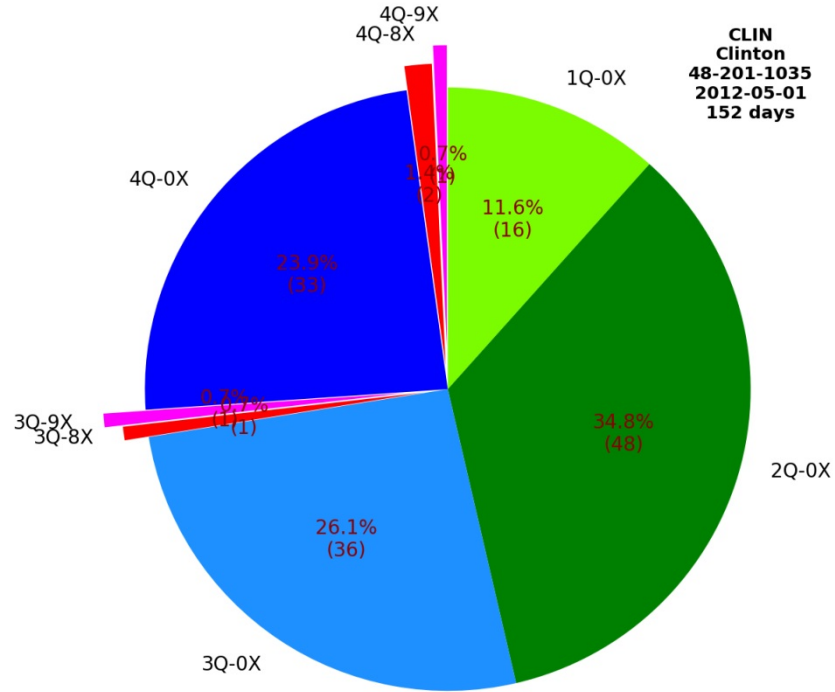
Predicted Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)



1X days are rank 1-15 annual days with O31H >= 100 ppb
8X days are rank 1-20 annual days with O38H >= 70 ppb
9X days have both 1X and 8X exceedances

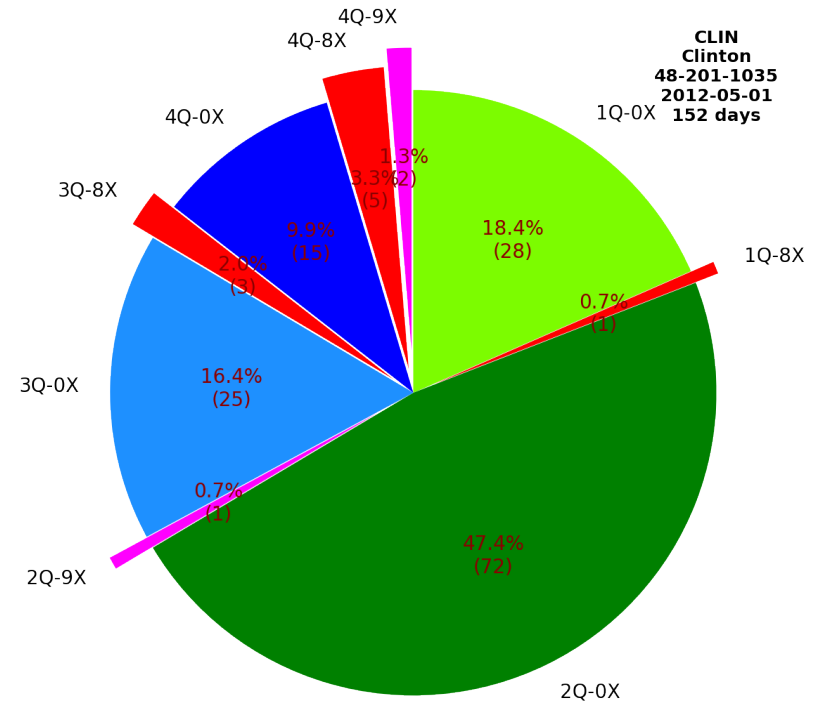
2012 CLIN Observed and Model Predicted Wind Quadrants and O₃ Exceedances

Observed Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)



1X days are rank 1-15 annual days with O₃1H >= 100 ppb
 8X days are rank 1-20 annual days with O₃8H >= 70 ppb
 9X days have both 1X and 8X exceedances

Predicted Wind Quadrants (Q) and O₃ 1-H and 8-H Exceedances (X)



1X days are rank 1-15 annual days with O₃1H >= 100 ppb
 8X days are rank 1-20 annual days with O₃8H >= 70 ppb
 9X days have both 1X and 8X exceedances

2012 Observed and Model Predicted Wind Quadrants and O₃ Exceedances Errors

Site H03H 2012 Wind nQ and Ozone nX Errors (days)

	Obs		Mod		Errors	
nQ	nObs	nX	nObs	nX	nQ	nX
-Q	1					
1Q	11	0	32	1	21	1
2Q	53	0	70	5	38	5
3Q	45	1	29	1	-16	0
4Q	42	4	21	4	-21	0
Days	152	5	152	11	22	6

Site CLIN 2012 Wind nQ and Ozone nX Errors (days)

	Obs		Mod		Errors	
nQ	nObs	nX	nObs	nX	nQ	nX
-Q	14					
1Q	16	0	29	1	13	1
2Q	48	0	73	1	25	1
3Q	38	2	28	3	-10	1
4Q	36	3	22	7	-14	4
Days	152	5	152	12	27	7

For 2012, the model predicts:

at H03H : 22 extra days with 1Q & 2Q days

at CLIN : 27 extra days with 1Q & 2Q days

For 2012, the model predicts:

at H03H : 6 more exceedance days

at CLIN : 7 more exceedance days

Further Investigation of the TCEQ CAMx Simulation IS PLANNED

- Common model performance issue :
 - **COMPENSATING ERRORS** across different processes components in model.
 - NASA/NOAA atmospheric researchers already found likely over-estimation of NO_x / CO emissions by 8-20% in the Model Inventories.

Reactive Source Areas

The low frequency of producing O_3 as demonstrated by the small ratio of 8X or 9X days compared to the much larger number of 3Q or 4Q 'necessary' conditions days for making O_3 , implies that there is a limit on the "sufficient" causes of 8/9X O_3 levels; that is, the reactive ingredients are not available often enough under 3/4Q conditions to result in more X's. The 'sufficient' causes must be NO/NOx and VOCs (that are not rapidly dispersed by 1Q or 2Q winds).

Further, the strength of the NOx source is highly repeatable as morning and evening traffic (and heavy duty trucks). (The NOx is a 'made' by-product of these activities). VOCs on the other hand are mostly *brought* in as liquid or gas, *STORED*, and can be vented or leaked to the atmosphere.

Biggest Issue Remaining : VOC levels and sources

- VOC measurements are not available for 2012
- VOC measurements (speciated) available part of 2016 at BULL
- Model VOCs are based on `ozone season' average inventories, lacking any `short-term' or accidental daily or hourly information. Model uses small number of `model VOC species'
- Based on significant experience in Houston (beginning in 2003) other ways to `see' rapid emissions of ozone forming VOCs was and is the `Infra Red Camera' which resulted in removing numerous small (but `plume' like) varying sources that could be traced to ozone production.

The Sensitivity to Visualize Even Small Leaks

With its superior resolution, thermal sensitivity, and the option of a High Sensitivity Mode, the FLIR GFx320 allows you to visualize leaks so you can pinpoint the exact source of the emissions and begin repairs immediately. In addition, the GFx320 can accurately measure temperatures, allowing you to note temperature differentials and improve visual contrast for better gas plume detection.



National Physical Laboratory (NPL) reports that through independent testing, it demonstrated the FLIR GF320 is capable of detecting gas emissions according to the standards set in the Environmental Protection Agency's (EPA) NSPS 40 CFR part 60, subpart 0000a sensitivity standard for optical gas imaging equipment.

IR Camera View of Storage Tanks in Houston.





Summary Findings

- Rotating wind flows **`necessary`** for ozone exceedances (confirmed by site data)
 - SANA wind Q-pie charts nearly identical to Houston for 2012, 2015, 2016, but differ by year.
- Hypothesize that Reactive Source Areas are source of **`sufficient`** VOCs
 - Strongly supported by morning wind direction and travel distance scatter plots.
 - Morning wind directions at BULL sites are from the W-NW and NW-N and at SANW are from NW-N for 8x and 9x ozone days and very rare from SE-S, toward the city core.
 - Site NOx poorly correlated with site 8-H or 1-H peak ozone.
 - Propose the use of IR-Camera to detect small, perhaps irregular, VOC sources.
- TCEQ CAMx Model 2012 shows significant discrepancies for **`rotating winds`** and for number of predicted ozone exceedance days at two Houston monitoring sites (preparing San Antonio model data for same tests)
 - Model incorrectly overpredicts exceedances for daily 1-quadrant and 2-quadrant winds.
 - Comparison of 2 Houston sites with TCEQ CAMx Model of 2012 shows model predicts significant differences in the distribution of wind quadrants and overpredicts the number of O3 exceedances by 6 and 7 more days as exceeding.

Ozone attainment action plan update

- Ozone Attainment Plan Construction
- Communications
- VW Beneficiary Mitigation Plan
- Current Initiatives/Recommendations
- ID Point Sources & Mitigation
- Business Involvement
- Policy/Advocacy/Funding



Underway

- Departmental ozone action plans updated
- VW Settlement coordination
- Meetings with business groups
- TCEQ presentations on non-attainment
- Monthly meetings with EPA/TCEQ/Bexar County
- RFI to identify VOC sources/species
- Synergy between Ozone Attainment and Climate Action



Next Steps

San Antonio/Bexar County
Ozone Attainment Plan Due
March 2019



- Obtain stakeholder input
- Develop Communications Plan
- Identify VW Settlement projects
- Identify/implement best practices--best in class cities
- Research AQ funding and proposed legislation
- Engage business community on mitigation efforts
- Identify and begin mitigation of NOx and VOCs

Thank you. Any Questions?



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