NAQFC Emission upgrade & tested FV3 meteorology & wild-fire impacts

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Talk Outline

I. Emission Upgrade NEI2014 version 2 (January 2019) :
   a) MOVES2014 -- temperature dependence done FY17
   b) Area: Activity factor upgrades for:
      - agricultural
      - Rail
      - Classes I, II marine
      - Residential wood burning
   c) Point and area: Both categories assigned for oil and gas

II. 72 hr forecast :
   a) CMAQ5.0.2 driven by FV3 core
   b) Investigation on DAY3 accuracy

III. Chemistry with cb6 and aero6 and tested that for wild-fires :
   a) Investigate new chemistry with extended VOC, Halogen, OA
   b) Investigate new chemistry & wild-fires impact

Current Operations

I. CMAQ4.7 (cb5 and aero4 – 103 species) for AK and HI:
   - Rather old, too efficient production of O_3 by NTR (organic nitrate).

II. CMAQ5.0.2 (cb05 and aero6 – 155 species) for CONUS:
   - Explicitly modeling NTR by various alkyl nitrates species
   - Improved dust and PM modeling by adding 17 mineral species

Developmental runs:

CMAQ5.2 for CONUS with fire gas-chemistry and smoke LBC

- SOA module and BEIS with enhanced summer time production of SOA
- CB6 and aero6 – 228 species: Advancement VOC chemistry & Combustion PM
- Photolysis rate attenuation from aerosol diming
- Halogen chemistry: Cl, Br, and I
- Account gas-chemistry by adopting EPA smoke-2-cmaq chemical profile
- LBC from operational NGAC for intruding smoke plume species

Prod-configuration

Emission for Prod (CMAQ5.0.2)

- **Point sources**: upgrade based on 2017 CEM and 2018 DoE Energy Outlook
  Canada 2011 Environment Canada Emission Inventory (ECEI);
  Mexico inventory (MI) 2012 version2.2
- **Area sources**: NEI2011 with O_n_G adjustment for 2016 + FORM/NOx upgrade,
  non-road: for U.S. used NEI2011, ECEI 2006 for Canada; MI 2012 for Mexico
- **Mobile sources**: Cross State Air Pollution Rule (CSAPR) 2011 Emission Data
- **Intermittent emissions:** windblown dust – FENGSHA Model (Tong et al., 2016)
- **wild fires** -- NESDIS Hazard Mapping System (HMS) & fuel from New USFS
  BlueSky v3.5.1
- **Natural source**: Biogenic with BEIS3 Version 3.14; Sea-salt based on 10m wind

FV3-CMAQ5.0.2 MDA8 O_3 Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
CON (N=13720) D1	37.8	5.56	15.3	9.76	0.82	0.86
D2		4.91	13.0	9.54	0.78	0.84
D3		4.75	12.6	9.77	0.76	0.83
R1 (N=650) D1	29.3	7.56	26.78	9.97	0.74	0.73
D2		8.44	28.80	10.83	0.60	0.60
D3		8.99	30.68	11.54	0.53	0.53
R2(N=165) D1	27.1	7.55	28.38	9.79	0.78	0.76
D2		8.51	31.30	11.30	0.63	0.67
D3		10.86	39.95	13.00	0.63	0.62
R3(N=1645) D1	30.5	6.54	22.00	9.14	0.83	0.83
D2		6.18	20.16	9.79	0.70	0.75
D3		6.85	22.34	10.33	0.69	0.73

FV3-CMAQ5.0.2 MDA8 O_3 Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
R4 (N=1930) D1	35.5	4.00	10.88	8.40	0.85	0.88
D2		3.55	9.16	8.37	0.75	0.82
D3		3.32	8.57	8.48	0.74	0.82
R5 (N=2145) D1	37.5	7.56	26.78	9.97	0.74	0.73
D2		8.44	28.80	10.83	0.60	0.60
D3		8.99	30.68	11.54	0.53	0.53
R6(N=1545) D1	36.4	7.36	20.65	11.09	0.79	0.81
D2		6.77	18.33	10.75	0.76	0.81
D3		6.37	17.24	11.16	0.70	0.77
R7(N=495) D1	40.7	4.77	12.24	8.51	0.79	0.83
D2		4.23	10.25	7.81	0.68	0.75
D3		4.51	10.95	7.86	0.69	0.76

FV3-CMAQ5.0.2 MDA8 O_3 Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
R8 (N=980) D1	41.5	5.83	14.25	10.50	0.67	0.73
D2		5.11	12.19	9.97	0.67	0.73
D3		4.96	11.84	9.99	0.66	0.73
R9 (N=2380) D1	48.2	2.84	5.95	10.38	0.71	0.83
D2		1.48	3.00	9.50	0.69	0.82
D3		0.93	1.88	9.38	0.69	0.82
R10(N=280) D1	30.3	3.01	10.44	6.86	0.67	0.79
D2		2.89	9.38	6.78	0.52	0.68
D3		2.61	8.47	6.79	0.51	0.69

FV3-CMAQ5.0.2 MDA8 O_3 Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
CON (N=13720) D1	**37.8**	**5.56**	**15.3**	**9.76**	**0.82**	**0.86**
D2		**4.91**	**13.0**	**9.54**	**0.78**	**0.84**
D3		**4.75**	**12.6**	**9.77**	**0.76**	**0.83**

NMMb-CMAQ5.0.2 MDA8 O_3 Day1,2,3 for August 2017

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
CON (N=23150) D1	**38.1**	**3.43**	**9.0**	**9.49**	**0.66**	**0.77**
D2		**4.90**	**12.7**	**11.01**	**0.48**	**0.66**
D3		**2.24**	**5.83**	**10.36**	**0.52**	**0.70**

FV3-CMAQ5.0.2 24 h $PM_{2.5}$ Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
CON (N=9780) D1	6.5	2.10	32.20	6.72	0.42	0.58
D2		1.54	23.78	6.33	0.43	0.59
D3		1.04	16.05	6.21	0.43	0.60
R1 (N=465) D1	4.26	2.73	64.04	4.93	0.31	0.48
D2		1.89	44.39	4.56	0.34	0.51
D3		0.88	20.57	4.27	0.30	0.51
R2(N=120) D1	6.4	-0.36	-5.64	3.78	0.36	0.62
D2		-0.68	-10.58	4.42	0.22	0.54
D3		-2.04	-31.32	4.70	0.21	0.52
R3(N=605) D1	5.7	1.46	25.40	3.52	0.56	0.71
D2		0.39	6.83	4.04	0.37	0.61
D3		-0.84	-14.73	3.85	0.34	0.61

FV3-CMAQ5.0.2 24 h $PM_{2.5}$ Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
R4 (N=1170) D1	7.7	1.49	19.17	5.08	0.52	0.66
D2		1.05	13.55	4.92	0.52	0.67
D3		0.38	4.95	4.96	0.47	0.65
R5 (N=1230) D1	7.6	5.28	68.27	8.03	0.54	0.56
D2		4.85	64.33	7.91	0.60	0.58
D3		4.49	59.37	8.20	0.60	0.59
R6(N=860) D1	7.2	-0.61	-8.46	4.98	0.40	0.64
D2		-1.01	-13.92	4.81	0.42	0.65
D3		-1.38	-19.04	4.85	0.42	0.64
R7(N=330) D1	7.8	3.98	50.52	6.67	0.45	0.54
D2		3.55	45.31	6.65	0.49	0.58
D3		3.56	42.84	6.87	0.53	0.59

FV3-CMAQ5.0.2 24 h $PM_{2.5}$ Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
R8 (N=880) D1	6.6	1.96	29.24	8.99	0.49	0.63
D2		1.25	18.87	8.25	0.48	0.64
D3		0.93	13.90	8.10	0.43	0.62
R9 (N=1500) D1	7.4	-0.82	-11.13	3.44	0.62	0.78
D2		-1.04	-14.03	3.34	0.64	0.77
D3		-1.22	-16.50	3.49	0.61	0.75
R10(N=1550) D1	5.0	1.08	21.26	4.85	0.34	0.55
D2		0.60	11.86	4.49	0.34	0.57
D3		0.35	6.82	4.47	0.33	0.56

FV3-CMAQ5.0.2 24 h $PM_{2.5}$ Day1,2,3 for September 11-22 2018

	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
CON (N=9780) D1	**6.5**	**2.10**	**32.20**	**6.72**	**0.42**	**0.58**
D2		**1.54**	**23.78**	**6.33**	**0.43**	**0.59**
D3		**1.04**	**16.05**	**6.21**	**0.43**	**0.60**

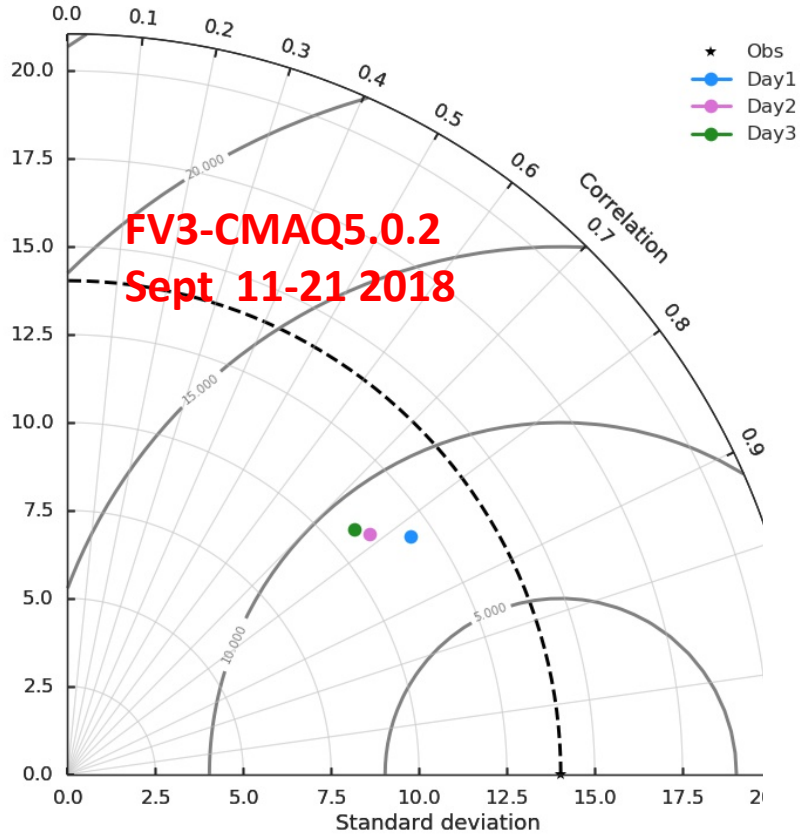
NMMb-CMAQ5.0.2 24 h $PM_{2.5}$ Day1,2,3 for August 2017

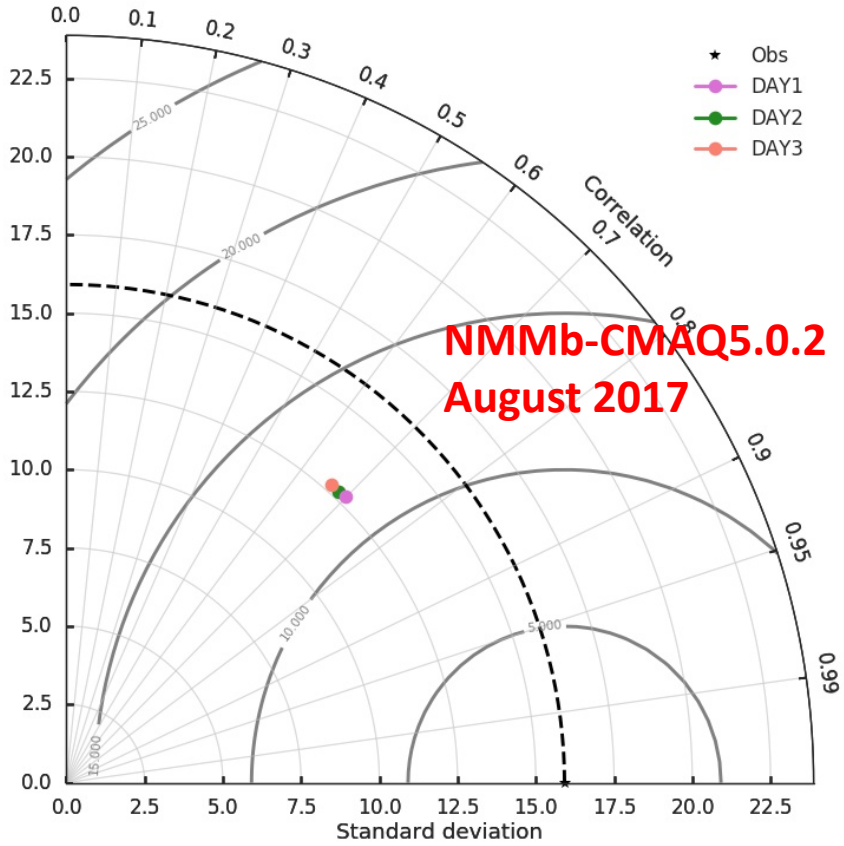
performance	obs	Bias	N-Mean B%	RMSE	corr, r	I Agreement
CON (N=14920) D1	**9.8**	**-0.44**	**-4.45**	**9.37**	**0.59**	**0.74**
D2		**-1.23**	**-12.55**	**14.23**	**0.51**	**0.66**
D3		**-0.28**	**-2.87**	**10.15**	**0.55**	**0.70**

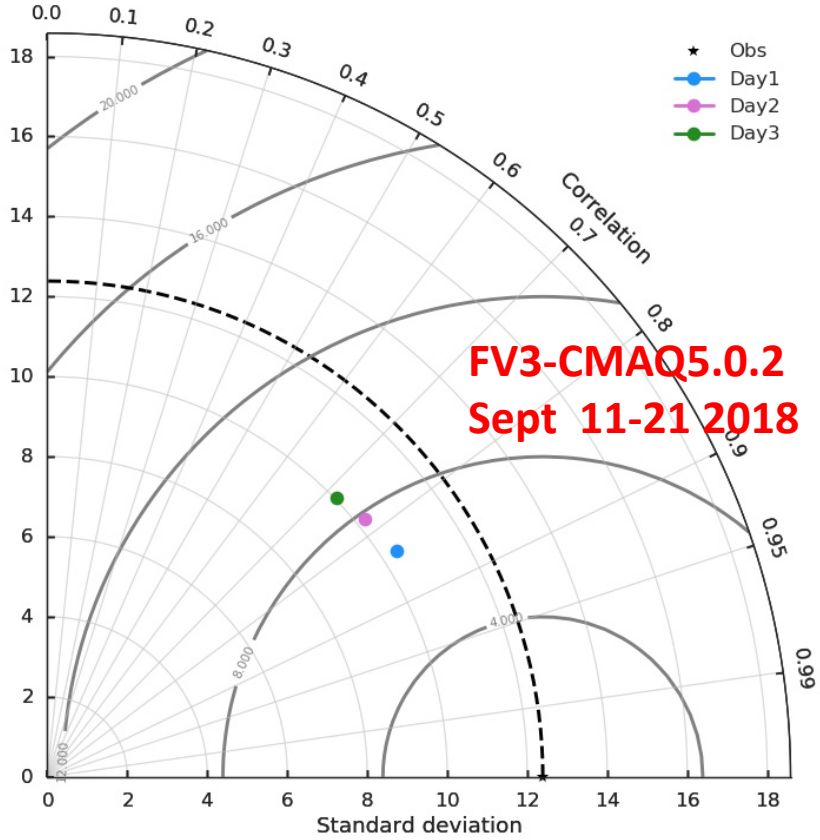
DAY3 accuracy of FV3-cmaq5.0.2 coupled system

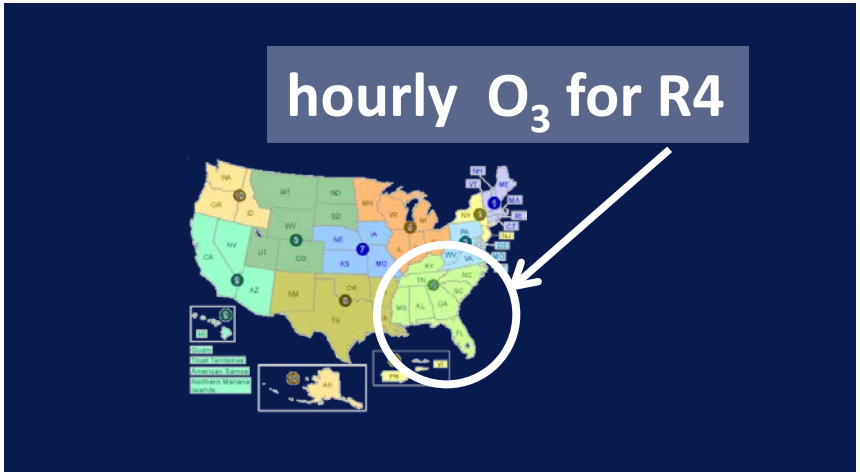
- Forecast accuracy deteriorates for Day2 and Day3
- Rate of deterioration does seem to increase over time
- MDA8 O_3:
  1. DAY2 was significantly less accurate than DAY1
  2. DAY3 further deteriorates from DAY2 but comparable
  3. Preliminary comparison between FV3- and NMMB-based systems showed FV3-based system better skill
- 24 hr $PM_{2.5}$:
  1. No clear trend of deterioration over time except Region 2 & 3 (Mid-Atlantic)?
  2. Test needed for diurnal distribution & fire impacts

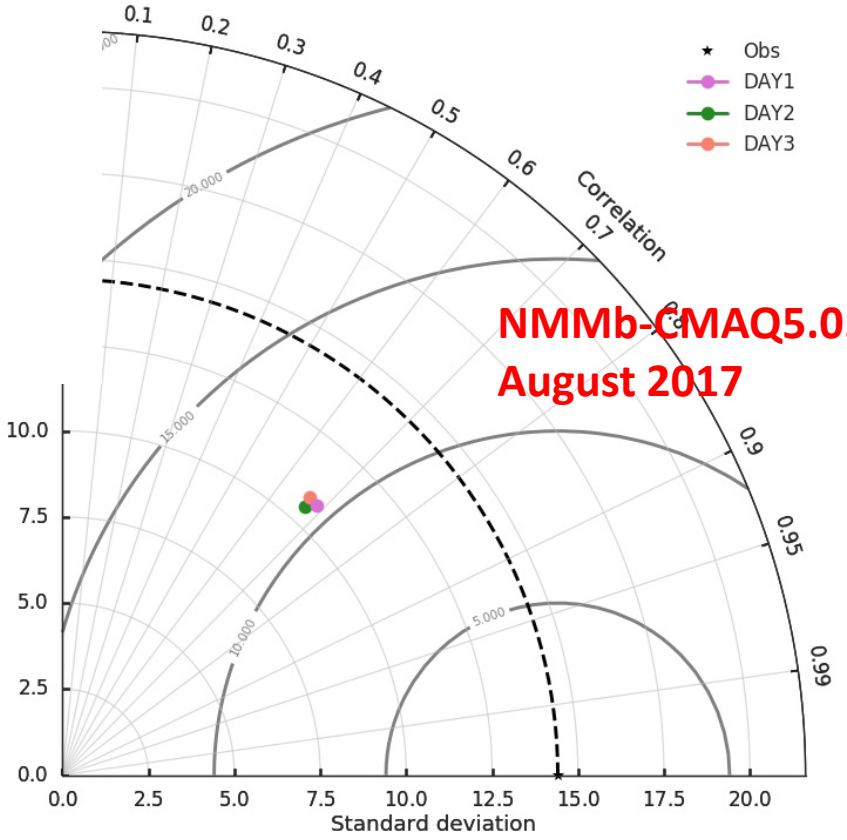
hourly O_3 for CONUS

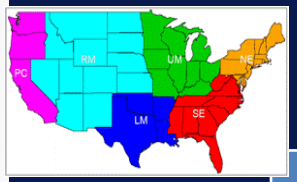





Obs
Day1
Day2
Day3
Correlation
Standard deviation
FV3-CMAQ5.0.2
Sept 11-21 2018


hourly O_3 for R4

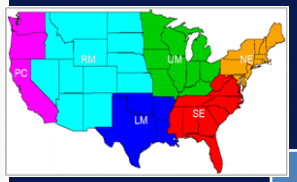

Obs
DAY1
DAY2
DAY3
Correlation
Standard deviation
NMMb-CMAQ5.0.2
August 2017



Performance NMM-CMAQ5.2 @ 20180916-20180919

Hourly averaged O_3

		N	obs	mean	Bias	RMSE	Coeff corr
5X	cmaq5.2	172600	26.1	34.8	8.71	14.17	0.71
	cmaq5.2 no fire			34.7	8.67	14.15	0.71
NE	cmaq5.2	22200	21.2	31.50	10.28	13.91	0.61
	cmaq5.2 no fire			31.50	10.31	13.93	0.61
SE	cmaq5.2	26600	22.1	34.30	12.13	15.92	0.72
	cmaq5.2 no fire			34.28	12.11	15.90	0.72
UM	cmaq5.2	37250	25.9	35.77	9.89	14.73	0.73
	cmaq5.2 no fire			35.75	9.88	14.73	0.73
LM	cmaq5.2	17400	25.6	35.85	10.23	15.01	0.77
	cmaq5.2 no fire			35.80	10.19	14.98	0.77
RM	cmaq5.2	28490	32.0	38.8	6.81	13.16	0.67
	cmaq5.2 no fire			38.7	6.71	13.10	0.67
CP	cmaq5.2	25480	33.3	35.70	2.38	12.71	0.72
	cmaq5.2 no fire			35.55	2.23	12.65	0.72

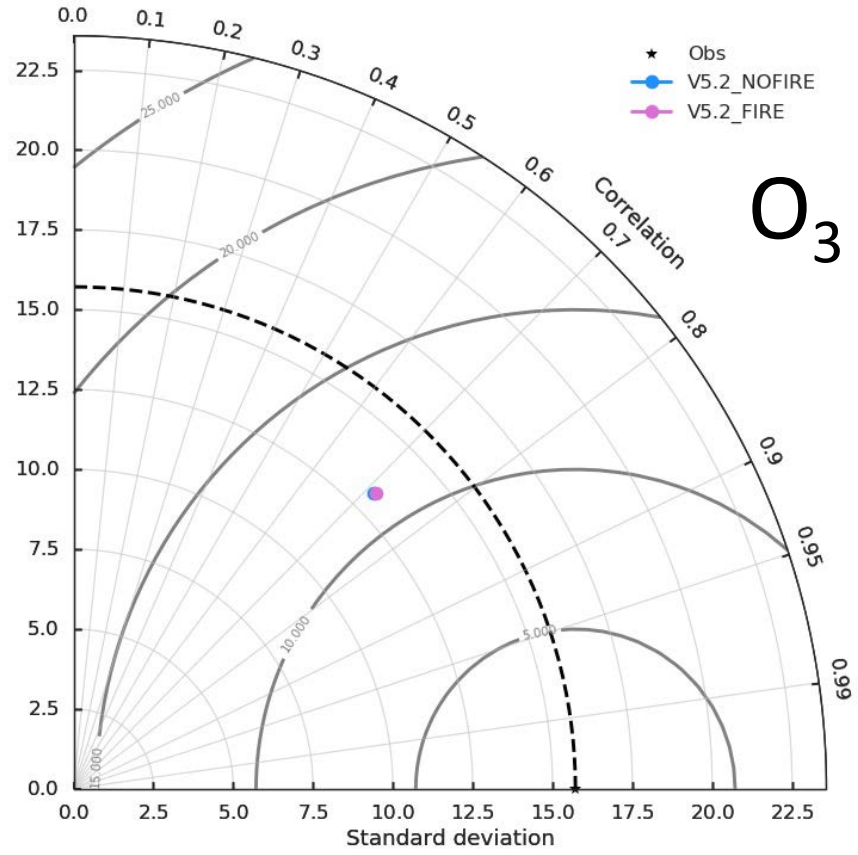


Performance NMM-CMAQ5.2 @ 20180916-20180919

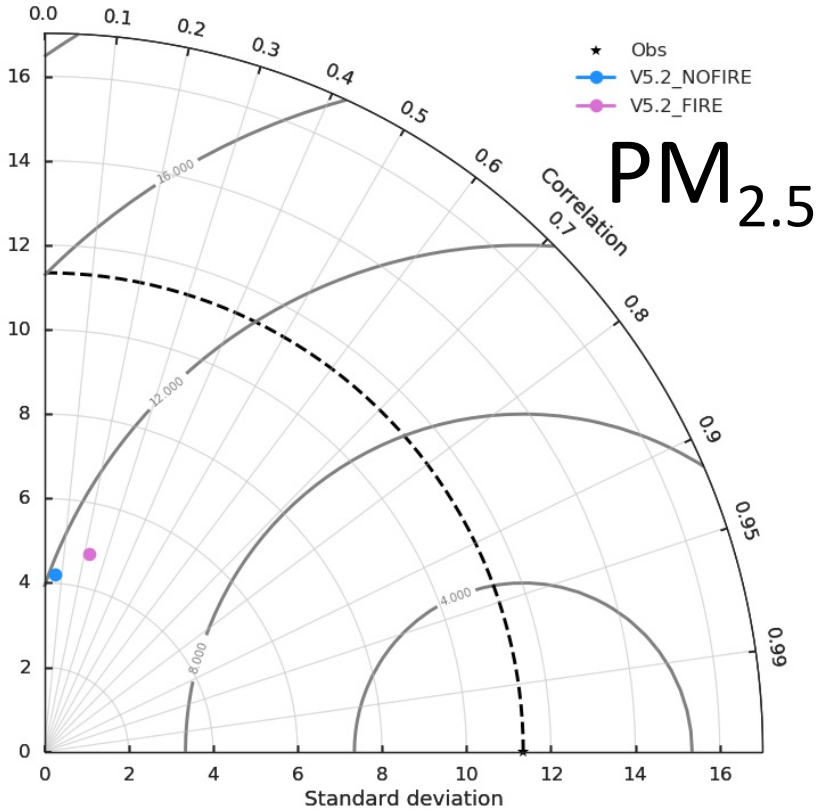
Hourly averaged $PM_{2.5}$

		N	obs	mean	Bias	RMSE	Coeff corr
5X	cmaq5.2	123800	6.7	11.18	4.48	11.03	0.37
	cmaq5.2 no fire			11.00	4.30	11.00	0.35
NE	cmaq5.2	14020	5.6	7.23	1.60	6.06	0.37
	cmaq5.2 no fire			7.19	1.56	6.03	0.37
SE	cmaq5.2	13570	7.4	13.30	5.84	10.83	0.45
	cmaq5.2 no fire			13.09	5.63	10.59	0.44
UM	cmaq5.2	20900	8.2	19.61	11.41	15.53	0.58
	cmaq5.2 no fire			19.44	11.25	15.35	0.58
LM	cmaq5.2	9730	9.0	15.88	6.86	13.18	0.56
	cmaq5.2 no fire			15.70	6.68	12.96	0.55
RM	cmaq5.2	21020	6.3	7.14	0.86	9.71	0.17
	cmaq5.2 no fire			6.75	0.48	10.07	0.07
CP	cmaq5.2	30630	6.3	7.00	0.69	6.62	0.31
	cmaq5.2 no fire			6.82	0.50	6.63	0.29

Taylor Diagram for CONUS Sep. 16-19 2018



O_3



$PM_{2.5}$

Wild-fire impact based on cmaq5.2: cb6 & aero6

- Study period is rather short: September 15-19 2018
- We aimed to test cb6 and aero6
- NEI2014v2 emission used --- same will be for NAQFC
- Hourly averaged O3:
  1. Wild-fire hardly increased any surface O3
- 24h PM2.5:
- It is advantageous to include full gas & aerosol chemistry
  1. A slight exacerbation of bias in over-prediction;
  2. Significant improvement in correlation.

Advantageous: gas & aerosol chemistry for PM2.5 forecast.

Summary

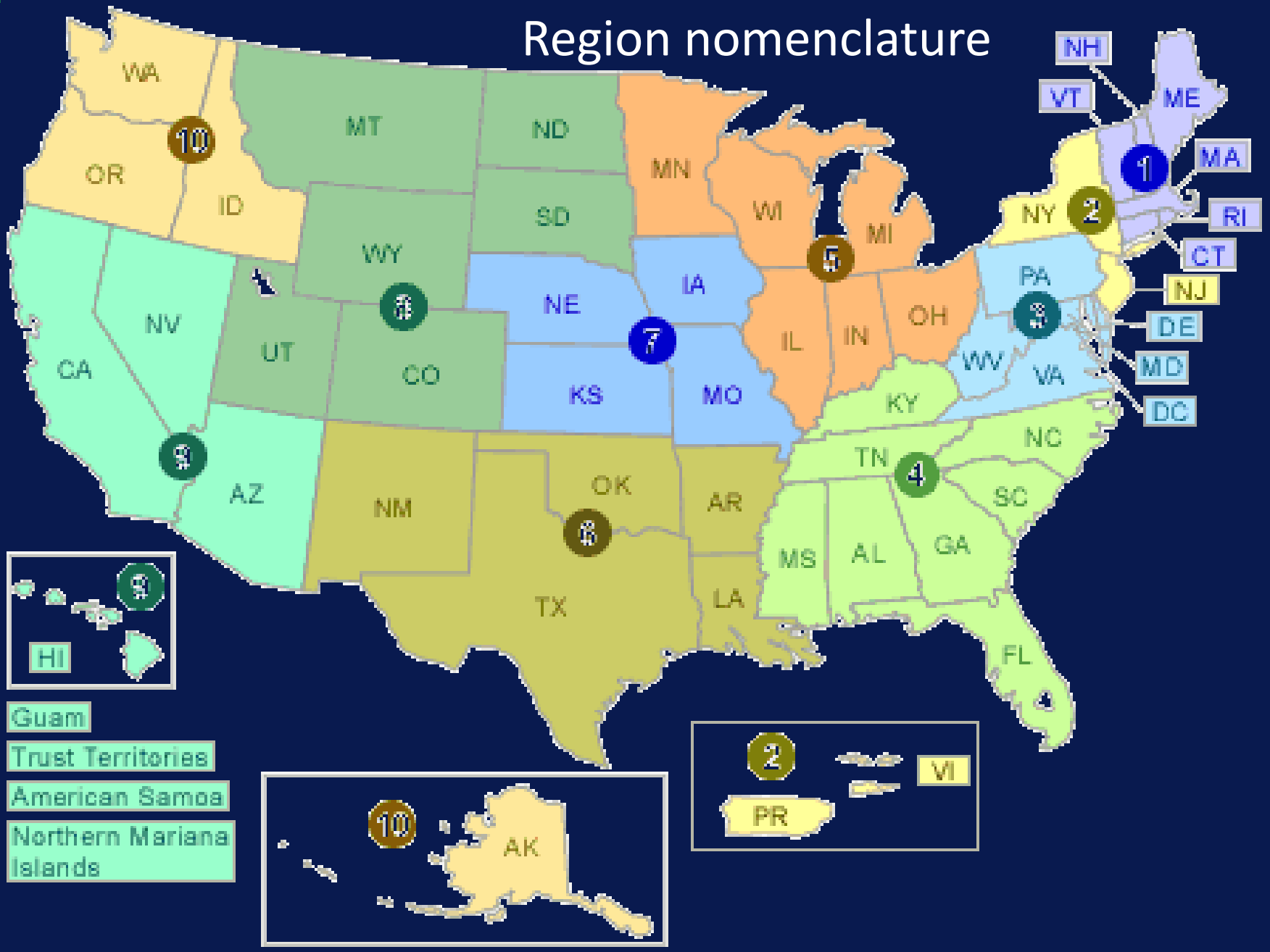
- Realized NEI2014v2 implementation;
- 72 hr forecast promising for O_3 but need work for $PM_{2.5}$;
- Testing with smoke LBC;
- Testing with smoke full-chemistry;
- Testing with cb6, aero6 paving way for in-line work and advanced science for Cl, BR,I and SOA impact on O_3 & $PM_{2.5}$.

Backup slide

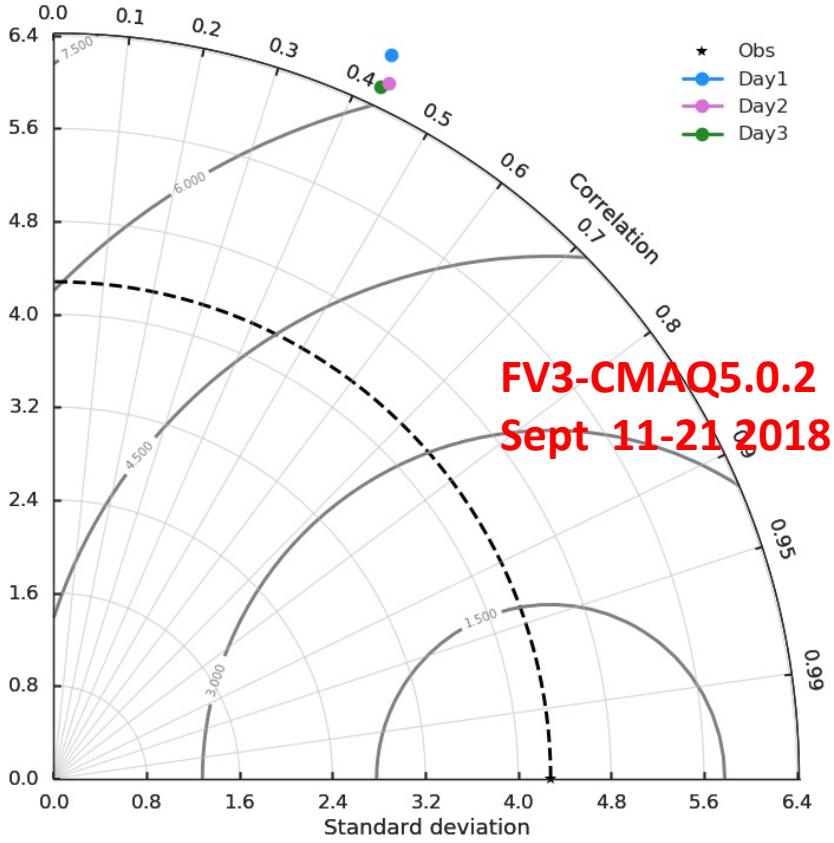
Emission NEI2014v2 OPS January 2019

Prod aqm	ARL Test bundle2 (CMAQ5.2)	Source Description
Mobile CSAPR	MOVES2014 version 2	EPA inventory & temperature dependence wrt 2017
Area:		
ag (NEI 2011)	ag (NEI 2014)	Agricultural NH3
afdust (2011)	afdust (2014)	Anthropogenic fugitive dust
alm (2011)	c1c2rail (2014)	Class I and I marine sources, railroad
	c3marine (none)	Class III marine sources (ocean going ships)
nr (2011)	nonroad (2014)	Nonroad (US)
nonpt (2011)	nonpt (2014)	Other area sources
othar (2011)	othar (2014)	Mexican and Canadian area sources
adjusted to 2016	np_oilgas (2014)	Non-point oil and gas sources
rwc (2011)	rwc (2014)	Residential wood combustion
Rail (N/A)	Rail (2014)	Dominantly from diesel engines
Point:		
ptnonipm	ptnonipm (2014)	Non-ipm point sources
N/A	pt_oilgas (2014)	Oil and gas point sources

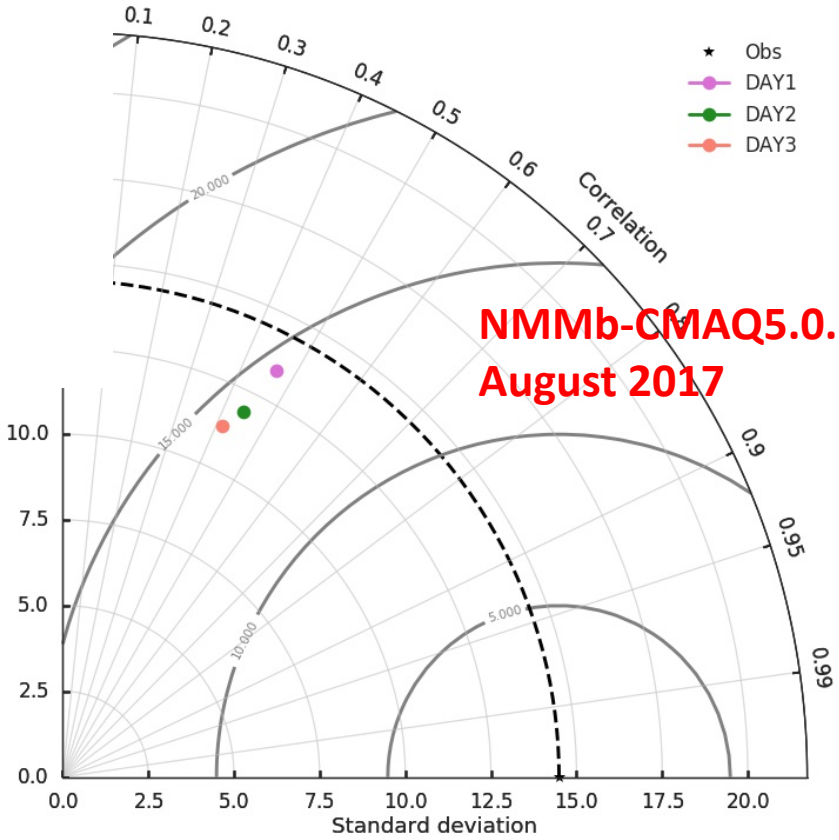
Region nomenclature



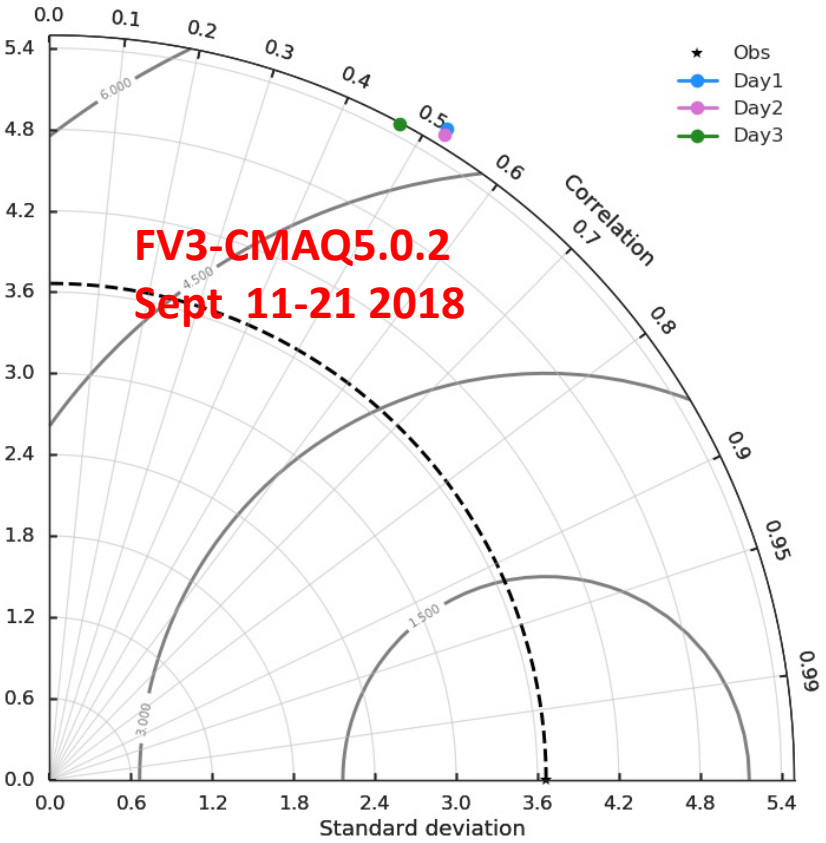
hourly $PM_{2.5}$ for CONUS

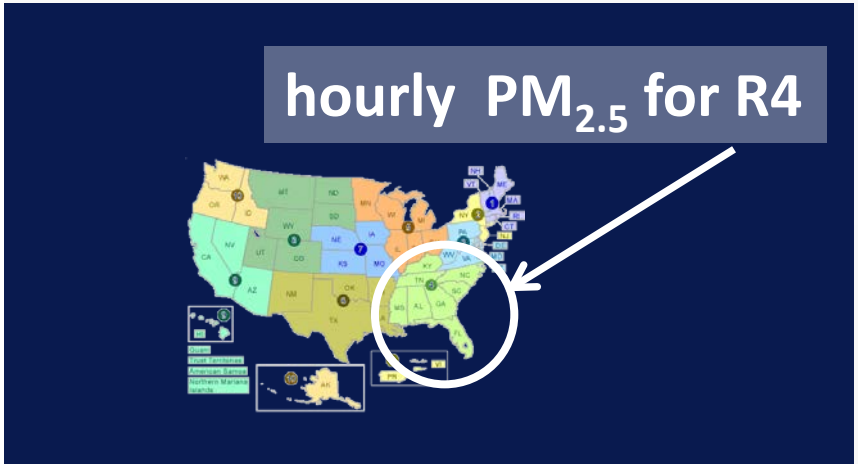


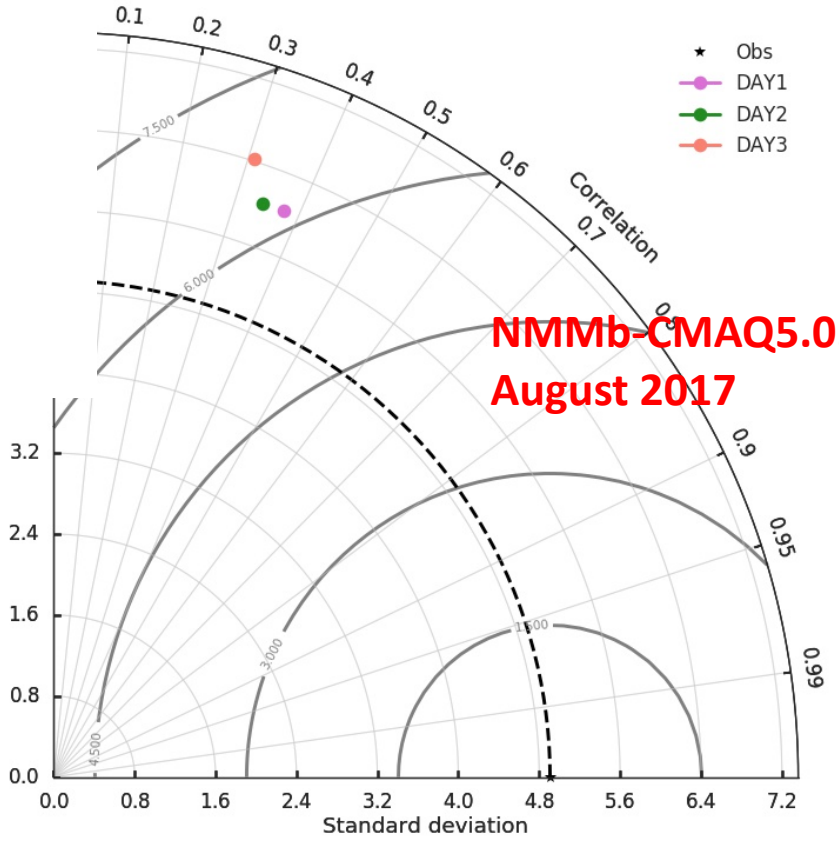
FV3-CMAQ5.0.2
Sept 11-21 2018



NMMb-CMAQ5.0.2
August 2017


Obs
Day1
Day2
Day3
Correlation
Standard deviation
FV3-CMAQ5.0.2
Sept 11-21 2018


hourly PM2.5 for R4


Obs
DAY1
DAY2
DAY3
Correlation
Standard deviation
NMMb-CMAQ5.0.2
August 2017