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Supplement of

Impacts of physical parameterization on prediction of ethane concentrations for oil and gas emissions in WRF-Chem

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S1. Definition of statistical measures

For quantitative comparison between the simulations we used statistical measures including correlation coefficient (R), root mean square error (RMSE), mean absolute error (MAE), mean bias (MB), and normalized mean bias (NMB). Definitions of these metrics can be found below:

$$R = \frac{\overline{(C_o - \bar{C}_o)(C_p - \bar{C}_p)}}{\sigma_{Cp}\sigma_{Co}} \quad (1)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (C_{p_i} - C_{o_i})^2}{n}} \quad (2)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |C_{p_i} - C_{o_i}| \quad (3)$$

$$MB = \frac{1}{n} \sum_{i=1}^n (C_{p_i} - C_{o_i}) \quad (4)$$

$$NMB = \frac{(\bar{C}_p - \bar{C}_o)}{\bar{C}_o} \times 100\% \quad (5)$$

Where C_o is the observation value, C_p is the model value, σ is the standard deviation, \bar{C} is the mean value, and n is total number of observation points

Table S1 Conversion table used to map species from NEI-2011 emission inventory to RACM chemical mechanism in and MADE/SORGAM aerosol module

Emission inventory name	WRF-Chem name	Weight	Species name
CO	e_co	1.00	Carbon monoxide
NOX	e_no	1.00	Nitrogen Oxides (NO or NO2)
SO2	e_so2	1.00	Sulfur dioxide
NH3	e_nh3	1.00	Ammonia
HC01	e_ch4	1.00	Methane
HC02	e_eth	1.00	Ethane kOH<500 /ppm/min
HC03	e_hc3	1.00	Alkane 500< kOH<2500 exclude(C3H8,C2H2,ethanol,acids)
HC04	e_hc3	1.11	Alkane 2500< kOH<5000 exlude(butanes)
HC05	e_hc5	0.97	Alkane 5000< kOH<10000 exlude(pentanes)
HC06	e_hc8	1.00	Alkane kOH>10000 exclude(ethylene glycol)
HC07	e_ol2	1.00	Ethylene
HC08	e_olt	1.00	Alkene kOH <20000 /ppm/min
HC09	e_oli	1.00	Alkene kOH >20000 /ppm/min exclude(dienes,styrenes)
HC10	e_iso	1.00	Isoprene
HC12	e_tol	1.00	Aromatic kOH <20000 /ppm/min exclude(benzene and toluene)
HC13	e_xyl	1.00	Aromatic kOH >20000 /ppm/min exclude(xylenes)
HC14	e_hcho	1.00	Formaldehyde
HC15	e_ald	1.00	Acetaldehyde
HC16	e_ald	1.00	Higher aldehydes
HC17	e_ald	1.00	Benzaldehyde
HC18	e_ket	0.33	Acetone
HC19	e_ket	1.61	Methylethyl ketone
HC20	e_ket	1.61	PRD2 SAPRAC species (aromatic ketones)
HC21	e_hc3	0.40	Methanol
HC22	e_ald	1.00	Glyoxal
HC23	e_ald	1.00	Methylglyoxal
HC24	e_ald	1.00	Biacetyl
HC25	e_csl	1.00	Phenols
HC26	e_csl	1.00	Cresols
HC27	e_ald	0.50	Methacrolein
HC27	e_olt	0.50	Methacrolein
HC28	e_ket	0.50	Methylvinyl ketone

HC28	e_olt	0.50	Methylvinyl ketone
HC29	e_ket	1.00	IPRD SAPRAC species (>C4 unsaturated aldehydes)
HC31	e_ora2	1.00	Acetic Acid
HC32	e_ora2	1.00	>C2 Acids (SAPRC PACD species)
HC33	e_csl	1.00	Xylenols (SAPRC-11 species)
HC34	e_csl	1.00	Catechols (SAPRC-11 species)
HC36	e_olt	1.00	Propylene
HC37	e_hc3	0.40	Acetylene
HC38	e_tol	0.29	Benzene
HC39	e_hc3	1.11	Butanes
HC40	e_hc5	0.97	Pentanes
HC41	e_tol	1.00	Toluene
HC42	e_xyl	1.00	m-Xylene
HC43	e_xyl	1.00	p-Xylene
HC44	e_xyl	1.00	o-Xylene
HC45	e_hc3	0.57	Propane
HC46	e_oli	1.00	Dienes
HC47	e_olt	1.00	Styrenes
HC47	e_tol	1.00	Styrenes
HC48	e_hc3	1.20	Ethanol
HC49	e_hc8	1.14	Ethylene Glycol
PM01	e_pm25i	0.20	Unspeciated primary PM2.5 - nuclei mode
PM01	e_pm25j	0.80	Unspeciated primary PM2.5 - accumulation mode
PM02	e_so4i	0.20	Sulfate PM2.5 - nuclei mode
PM02	e_so4j	0.80	Sulfate PM2.5 - accumulation mode
PM03	e_no3i	0.20	Nitrate PM2.5 - nuclei mode
PM03	e_no3j	0.80	Nitrate PM2.5 - accumulation mode
PM04	e_orgi	0.20	Organic Carbon PM2.5 - nuclei mode
PM04	e_orgj	0.80	Organic Carbon PM2.5 - accumulation mode
PM05	e_eci	0.20	Elemental Carbon PM2.5 - nuclei mode
PM05	e_ecj	0.80	Elemental Carbon PM2.5 - accumulation mode
PM10-PRI	e_pm10	1.00	Unspeciated Primary PM10

Table S2. Summary of model performance in capturing temperature at BAO 10m and 300m during Aug 1-15, 2014

T (C) - 10m	OBS	PBL			Met IC and BC		Initialization		Horizontal resolution	
		PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5- 12km
Mean	21.67	22.40	20.95	21.20	24.06	23.44	21.59	24.06	24.06	24.08
R	0.89	0.89	0.89		0.86	0.89	0.71	0.86	0.86	0.88
RMSE	2.05	2.03	2.01		3.25	2.63	2.99	3.25	3.25	3.18
MAE	1.56	1.62	1.59		2.60	2.05	2.30	2.60	2.60	2.53
MB	0.74	-0.72	-0.46		2.40	1.77	-0.08	2.40	2.40	2.41
NMB	3.4%	-3.3%	-2.1%		11.1%	8.2%	-0.4%	11.1%	11.1%	11.1%
T (C) - 300m	OBS	PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5- 12km
		21.91	20.95	21.30	23.58	22.89	20.31	23.58	23.58	23.52
Mean		0.76	0.75	0.72	0.74	0.78	0.57	0.74	0.74	0.75
R		2.16	2.14	2.10	2.79	2.27	3.09	2.79	2.79	2.80
RMSE		1.69	1.73	1.68	2.24	1.76	2.45	2.24	2.24	2.21
MAE		0.23	-0.73	-0.38	1.90	1.22	-1.37	1.90	1.90	1.85
MB		1.1%	-3.4%	-1.8%	8.8%	5.6%	-6.3%	8.8%	8.8%	8.5%

Table S3. Summary of model performance in capturing relative humidity (RH) at BAO 10m and 300m during Aug 1-15, 2014

RH (%) - 10m	OBS	PBL			Met IC and BC		Initialization		Horizontal resolution	
		PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5-12km
Mean	46.47	46.85	57.59	55.78	32.65	39.87	59.36	32.65	32.65	32.89
R	0.78	0.69	0.73	0.63	0.64	0.53	0.63	0.63	0.63	0.71
RMSE	10.89	16.90	15.13	19.13	14.95	22.33	19.13	19.13	19.13	18.15
MAE	8.45	14.38	12.86	15.01	11.31	18.10	15.01	15.01	15.01	14.43
MB	0.38	11.12	9.31	-13.81	-6.60	12.90	-13.51	-13.51	-13.51	-13.58
NMB	0.8%	23.9%	20.0%	-29.7%	-14.2%	27.7%	-29.7%	-29.7%	-29.7%	-29.2%
RH (%) - 300m	OBS	PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5-12km
		38.70	43.63	51.45	48.25	31.27	38.55	59.06	31.27	31.27
Mean		0.64	0.59	0.48	0.53	0.52	0.41	0.53	0.53	0.57
R		13.06	17.92	15.25	12.66	11.14	28.39	12.66	12.66	12.11
RMSE		9.92	14.78	12.77	9.73	8.60	23.19	9.73	9.73	9.29
MAE		4.93	12.75	9.55	-7.43	-0.15	20.36	-7.43	-7.43	-6.76
MB		12.7%	32.9%	24.7%	-19.2%	-0.4%	52.6%	-19.2%	-19.2%	-17.5%

Table S4 Summary of model performance in capturing wind speed and direction at BAO 10m during Aug 1-15, 2014

		PBL			Met		Init		Horizontal Res.		
Day - 10 m		OBS	PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5-12km
Wind Speed	Mean	2.46	2.99	2.68	2.20	2.63	2.83	3.30	2.63	2.63	2.58
	STD	1.25	1.47	1.55	1.27	1.41	1.51	2.02	1.41	1.41	1.33
Wind Direction	Mean	123.38	64.31	71.92	74.85	38.63	70.83	61.40	38.63	38.63	45.08
	STD	66.06	45.40	62.30	54.02	73.77	75.30	75.65	73.77	73.77	66.18
Night - 10 m		OBS	PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5-12km
Wind Speed	Mean	2.25	2.81	2.58	2.18	2.51	2.72	2.91	2.51	2.51	2.66
	STD	0.96	1.41	0.94	0.96	1.35	1.43	1.40	1.35	1.35	1.41
Wind Direction	Mean	222.98	244.07	243.95	263.07	226.97	230.93	160.02	226.97	226.97	295.43
	STD	50.01	90.68	69.52	74.66	83.89	69.81	87.15	83.89	83.89	87.30

Table S5 Summary of model performance in capturing wind speed and direction at BAO 300m during Aug 1-15, 2014

		PBL			Met		init		Horizontal Res.		
Day - 300 m		OBS	PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5-12km
Wind Speed	Mean	3.23	3.89	3.51	2.78	2.88	3.22	3.83	2.88	2.88	2.77
	STD	2.24	2.15	2.39	1.61	1.58	1.81	2.93	1.58	1.58	1.47
Wind Direction	Mean	117.31	62.69	62.42	64.05	32.91	57.67	56.71	32.91	32.91	39.52
	STD	74.56	51.99	63.89	59.84	75.14	76.03	74.32	75.14	75.14	69.43
Night - 300 m		PBL1	PBL2	PBL3	Met5	Met6	Init4	Init5	Hor5	Hor5-12km	
Wind Speed	Mean	3.42	5.00	4.34	3.80	4.21	4.60	5.07	4.21	4.21	4.89
	STD	2.59	2.68	2.95	2.64	2.64	2.47	3.07	2.64	2.64	3.29
Wind Direction	Mean Model	213.59	141.12	223.36	355.95	326.05	294.02	156.88	326.05	326.05	306.58
	STD Model	72.73	98.36	93.80	91.39	91.33	77.67	84.60	91.33	91.33	88.31

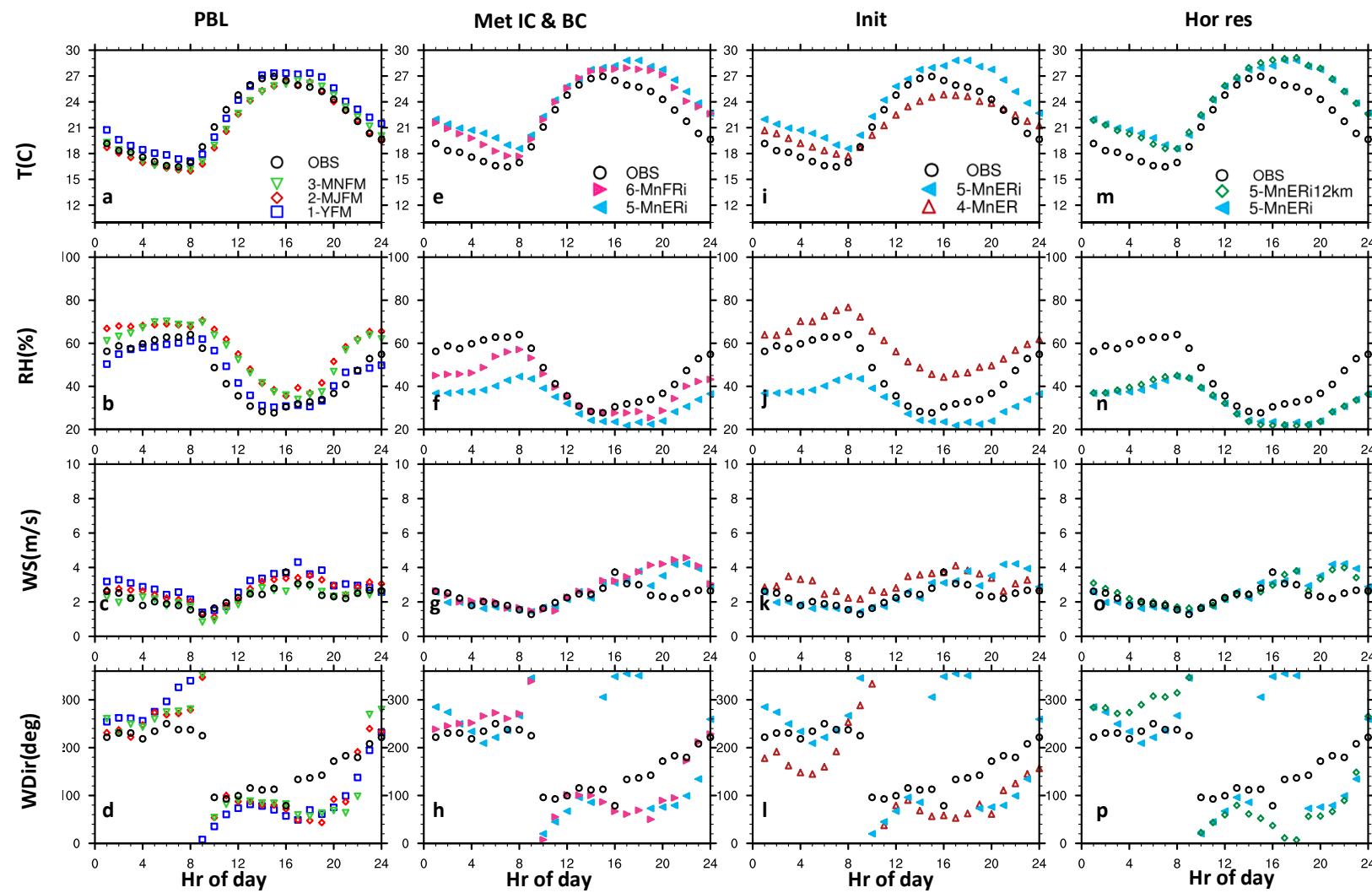


Figure S1 Average diurnal cycle of temperature, relative humidity, wind speed, and wind direction for all test sets and observation at BAO 10m. Averages are calculated for Aug 1 to 15, 2014

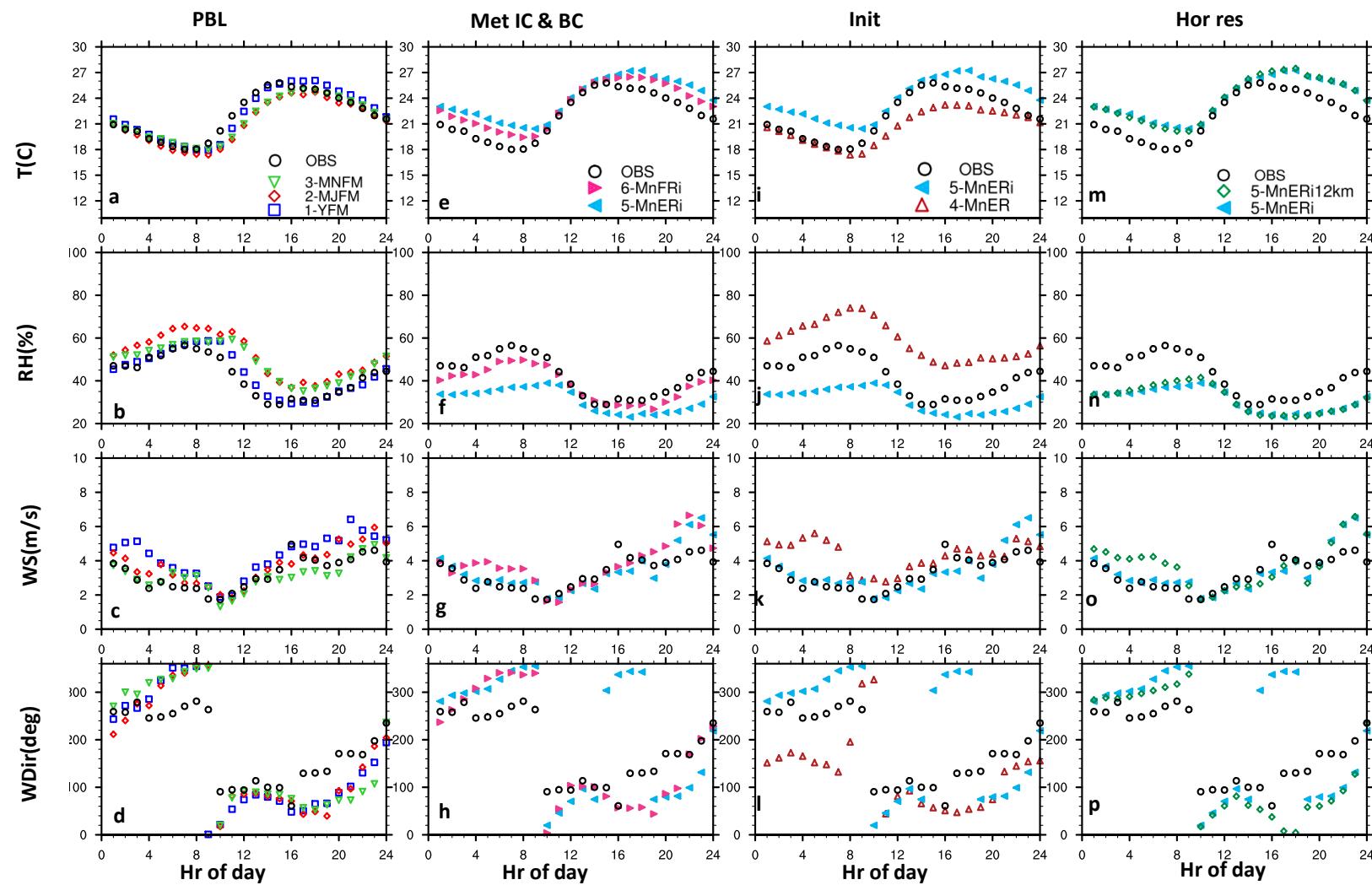


Figure S2 Average diurnal cycle of temperature, relative humidity, wind speed, and wind direction for all test sets and observation at BAO 100m. Averages are calculated for Aug 1 to 15, 2014

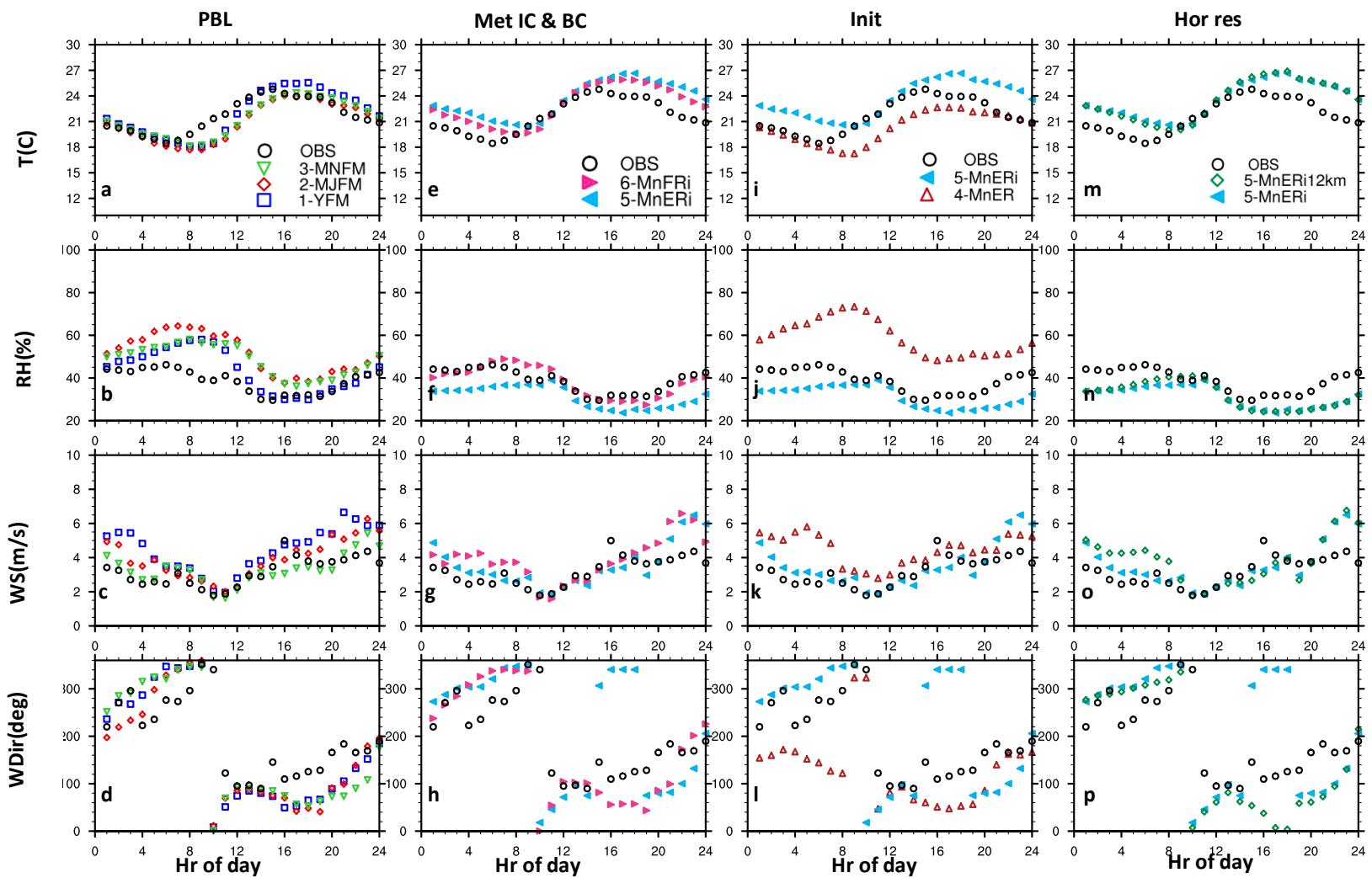


Figure S3 Average diurnal cycle of temperature, relative humidity, wind speed, and wind direction for all test sets and observation at BAO 300m. Averages are calculated for Aug 1 to 15, 2014

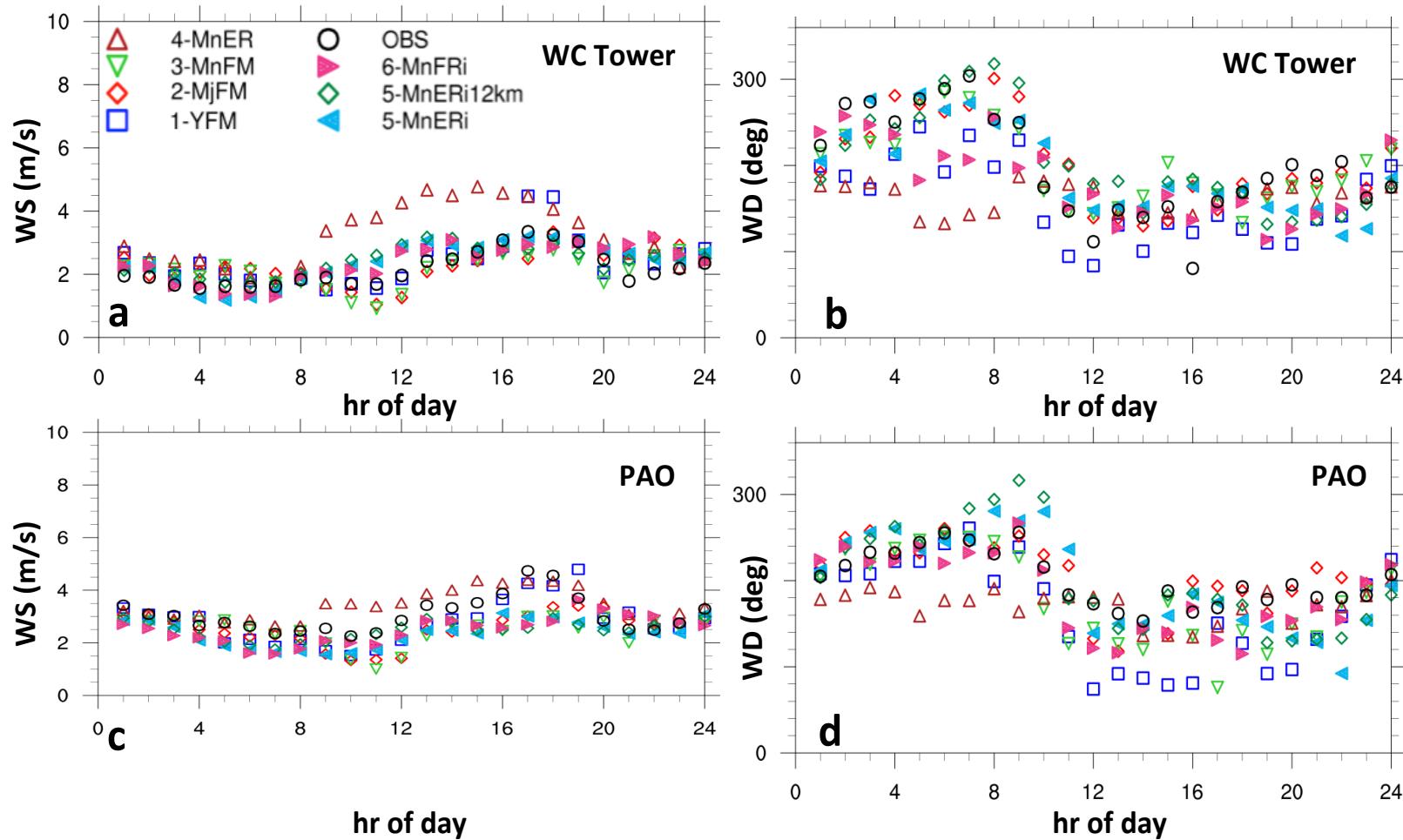


Figure S4. Average diurnal cycle of wind speed (WS) and direction (WD) at WC Tower and PAO sites. Averages are calculated for August 1 to 11, 2014

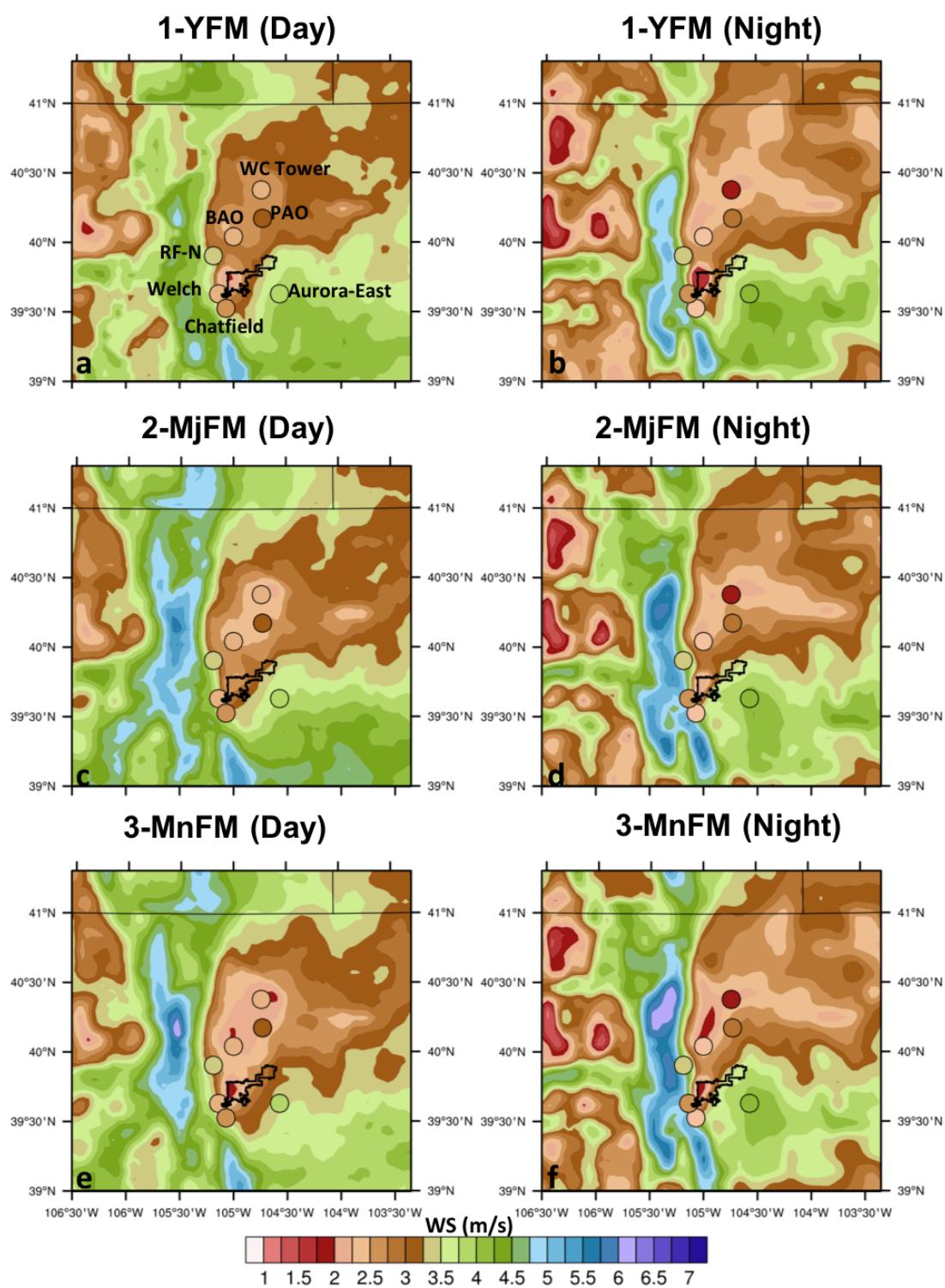


Figure S5 Wind speed at 10m captured by different PBL schemes. averaged from 1-August to 11-August 2014

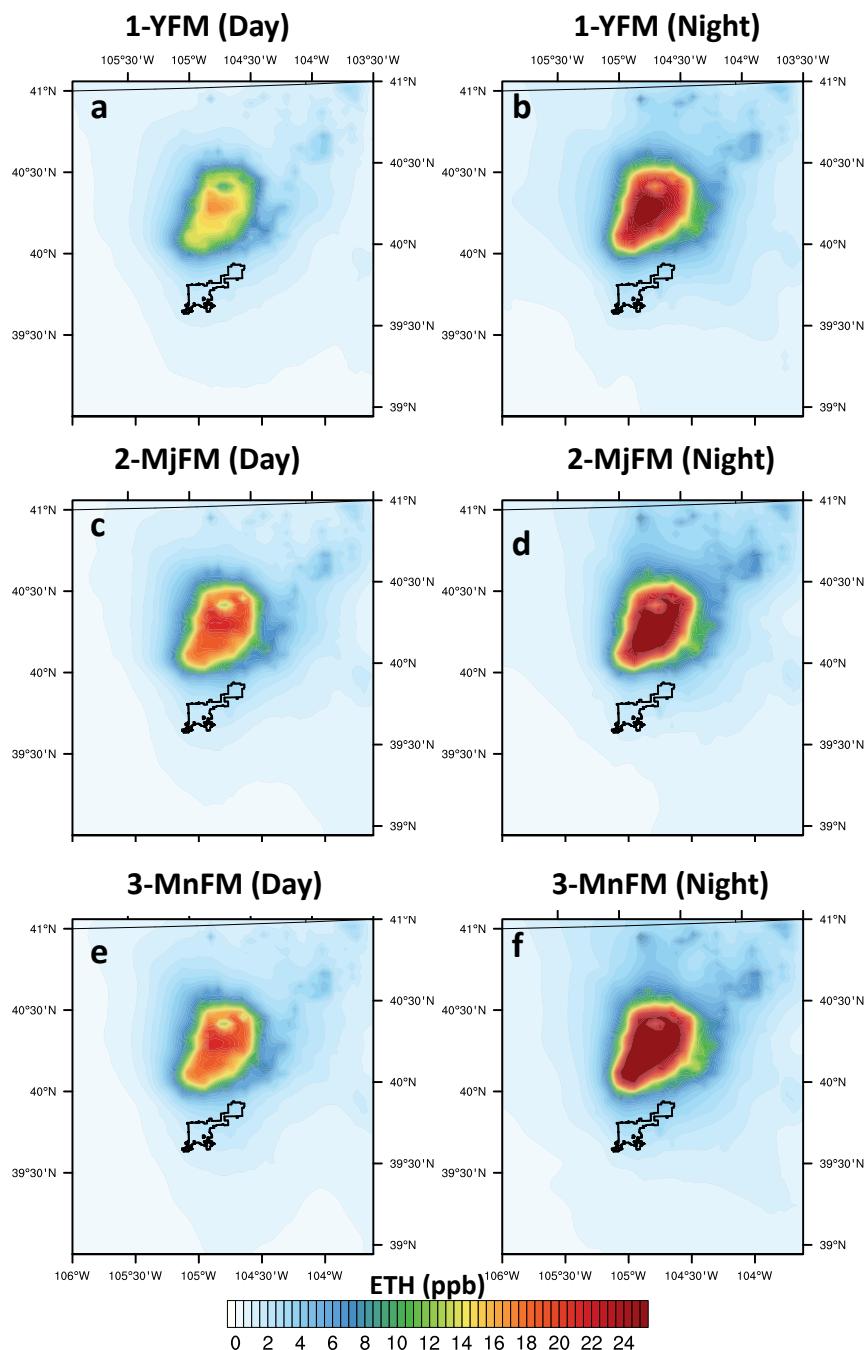


Figure S6. Surface ethane in sim 1 (1-YFM), sim 2 (2-MjFM), sim 3 (3-MnFm) averaged from August 1 to 15, 2014

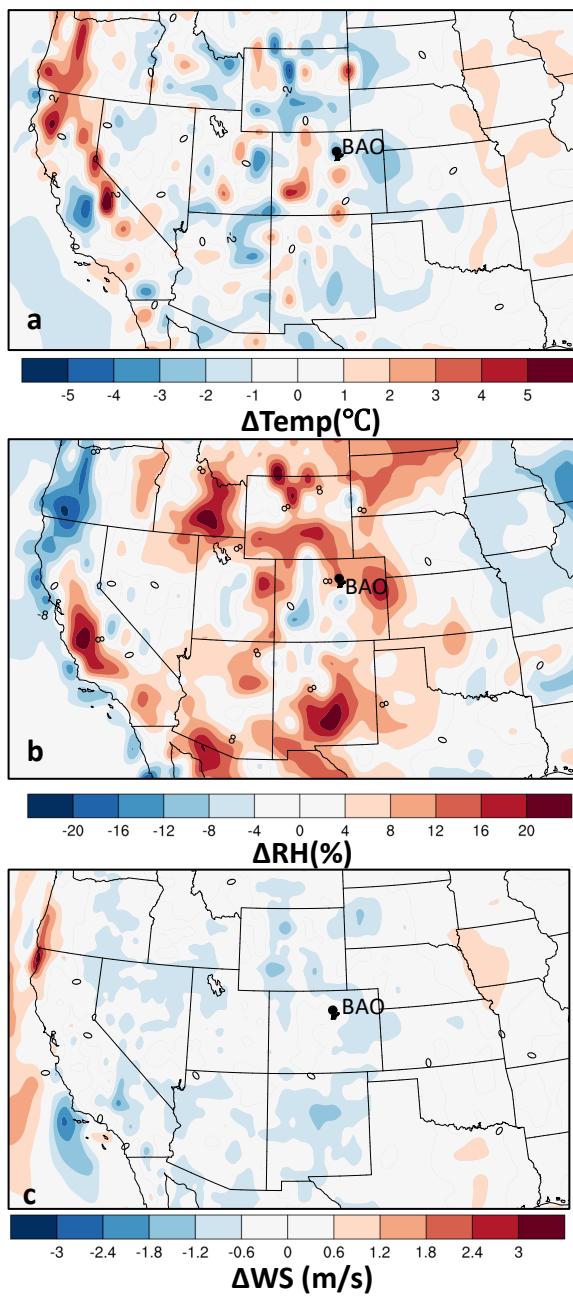


Figure S7 Differences in temperature (a), relative humidity (b), and wind speed (c) between ERA-interim and NCEP-FNL global models ($\Delta x = X(\text{ERA-interim}) - X(\text{NCEP-FNL})$) averaged from Aug 1 to 15, 2014 using 6-hourly data

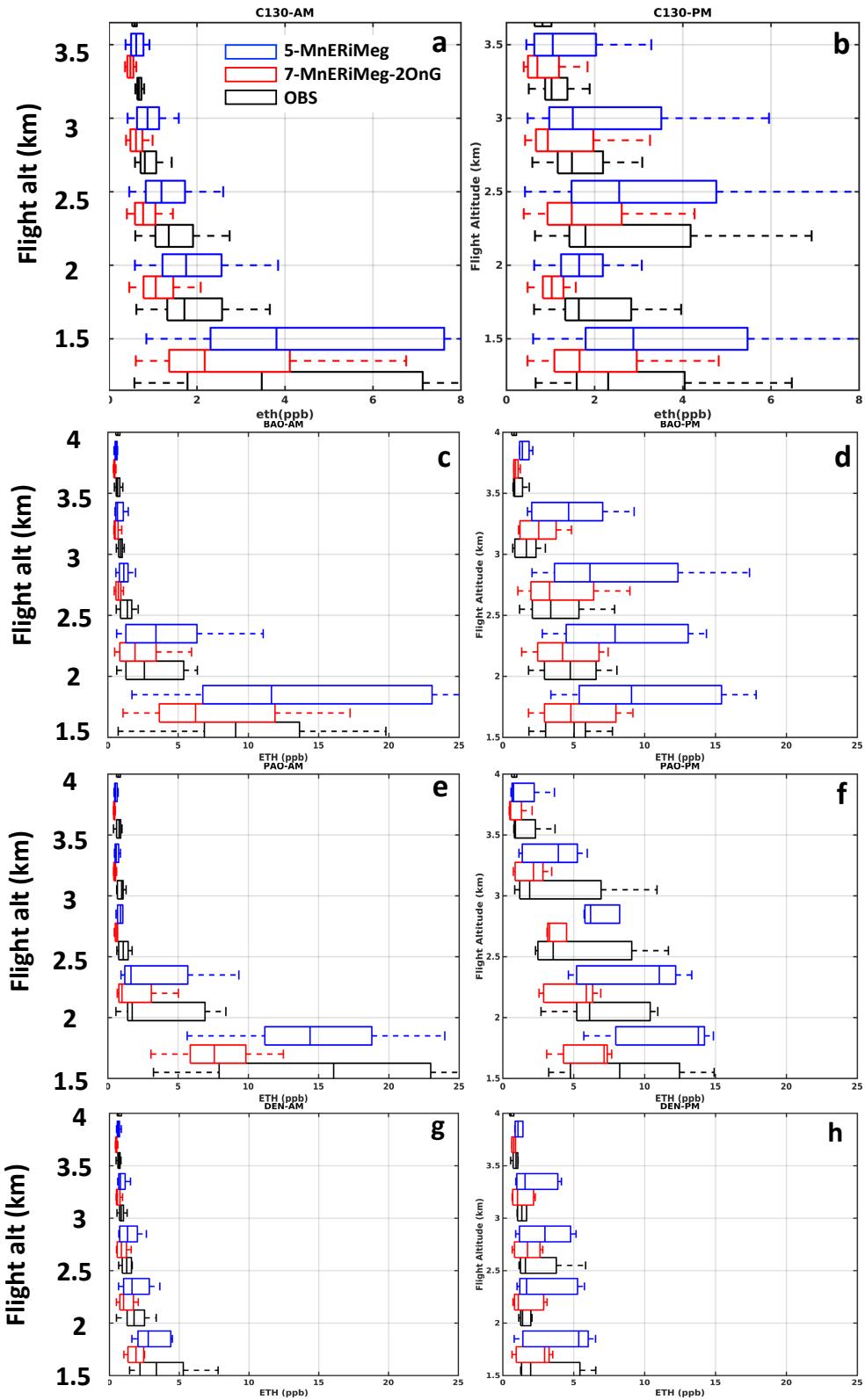


Figure S8. Sensitivity of ethane to oil and NG emission during C130-AM (a), C130-PM (b), P3-PAO AM (d), P3-PAO PM (c), P3-BAO AM (e), P3-BAO PM (f) averaged for August flights