

Supplemental Information for **Evaluation of Ozone and its Precursors using the Multi-Scale Infrastructure for Chemistry and Aerosols Version 0 (MUSICAv0) during the Michigan-Ontario Ozone Source Experiment (MOOSE)**

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Table S1: Total anthropogenic nitric oxide (NO) emissions from the CAMSv5.1 in Michigan and Southeast Michigan, and their ratio from various sectors*.

	MICH [kt]	SEMI [kt]	SEMI/MICH
AGS	0.46	0.04	9.0%
AWB	0.10	0.01	10.8%
ENE	9.44	2.86	30.3%
RES	1.03	0.48	47.1%
TNR	1.99	0.36	18.1%
TRO	15.13	3.50	23.2%

*AGS = Agriculture Soils; AWB = Agriculture Waste Burning;
ENE = Power Generation; RES = Residential; TNR = Off-Road
Transportation; TRO = Road Transportation

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Table S2: Mean biases (MB), root-mean squared errors (RMSE), and Pearson correlations (CORR) for surface O₃ concentrations compared to observations from available MI EGLE stationary sites (Model – Observations).

		MB	RMSE	CORR
Allen Park	ne30x8	-3.66	13.09	0.73
	ne30x8 DIUR	-2.32	12.10	0.73
	ne30x16	-6.38	13.64	0.72
	ne30x16 DIUR	-5.57	12.91	0.71
Detroit–E 7 Mile	ne30x8	0.17	13.17	0.72
	ne30x8 DIUR	1.74	12.54	0.72
	ne30x16	-2.60	13.17	0.71
	ne30x16 DIUR	-1.58	12.15	0.72
New Haven	ne30x8	0.89	11.28	0.77
	ne30x8 DIUR	2.38	11.67	0.76
	ne30x16	-0.85	11.56	0.75
	ne30x16 DIUR	-0.22	11.40	0.74
Oak Park	ne30x8	0.26	12.69	0.74
	ne30x8 DIUR	1.97	11.99	0.75
	ne30x16	-1.12	11.56	0.76
	ne30x16 DIUR	0.02	11.10	0.75
Port Huron	ne30x8	-3.12	12.57	0.72
	ne30x8 DIUR	-2.14	12.15	0.71
	ne30x16	-6.26	13.97	0.69
	ne30x16 DIUR	-5.57	13.63	0.67
Warren	ne30x8	2.55	12.67	0.74
	ne30x8 DIUR	4.09	12.32	0.75
	ne30x16	-0.52	12.12	0.73
	ne30x16 DIUR	0.47	11.32	0.73
Ypsilanti	ne30x8	3.69	10.92	0.77
	ne30x8 DIUR	5.63	11.46	0.78
	ne30x16	2.46	10.91	0.75
	ne30x16 DIUR	3.13	10.97	0.75

110 Table S3: Same as Table S2, but for NO₂.

		MB	RMSE	CORR
Detroit–E 7 Mile	ne30x8	2.48	6.25	0.61
	ne30x8 DIUR	1.93	5.14	0.59
	ne30x16	2.65	6.96	0.57
	ne30x16 DIUR	1.87	5.75	0.53
Detroit - SW	ne30x8	2.56	6.89	0.54
	ne30x8 DIUR	1.81	5.82	0.47
	ne30x16	3.85	8.12	0.56
	ne30x16 DIUR	2.94	7.13	0.48
DP4th	ne30x8	1.52	7.31	0.54
	ne30x8 DIUR	0.29	6.39	0.45
	ne30x16	3.67	8.31	0.54
	ne30x16 DIUR	2.67	7.40	0.46
Eliza Howell–NR	ne30x8	-10.32	12.81	0.05
	ne30x8 DIUR	-10.85	13.11	0.05
	ne30x16	-10.35	12.73	0.06
	ne30x16 DIUR	-10.83	13.03	0.06
Military Park	ne30x8	1.98	7.02	0.60
	ne30x8 DIUR	0.65	5.63	0.56
	ne30x16	4.13	8.31	0.57
	ne30x16 DIUR	3.03	6.95	0.54
Trinity St. Marks	ne30x8	1.98	7.31	0.41
	ne30x8 DIUR	1.38	6.01	0.41
	ne30x16	2.83	8.07	0.46
	ne30x16 DIUR	2.23	6.88	0.47

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Table S4: Pearson correlations (CORR), standard deviations (STD), normalized standard deviations (CV), root-mean squared errors (RMSE) and normalized root-mean squared errors (NRMSE) of the model simulations compared to available gas-phase chemical species from the Aerodyne Mobile Laboratory (AML).

		CORR	STD	CV	RMSE	NRMSE
O ₃	ne30x8	0.74	19.12	55.04	12.83	0.84
	ne30x8 DIUR	0.76	17.56	48.23	11.72	0.77
	ne30x16	0.74	17.86	56.65	12.91	0.85
	ne30x16 DIUR	0.73	15.98	48.82	11.84	0.78
HCHO	ne30x8	0.58	1.46	57.37	1.26	1.02
	ne30x8 DIUR	0.59	1.48	58.49	1.27	1.02
	ne30x16	0.61	0.91	45.55	1.07	0.86
	ne30x16 DIUR	0.58	0.91	44.93	1.1	0.89
NO	ne30x8	0.29	4.51	161.75	10.5	1.03
	ne30x8 DIUR	0.35	4	159.77	10.31	1.01
	ne30x16	0.3	6.13	169.44	10.55	1.04
	ne30x16 DIUR	0.32	5.03	168.98	10.36	1.02
NO ₂	ne30x8	0.46	7.99	63.76	8.07	1.1
	ne30x8 DIUR	0.49	5.71	50.37	6.73	0.92
	ne30x16	0.58	9.49	68.33	8.36	1.14
	ne30x16 DIUR	0.59	7.12	58.69	6.59	0.9
NO _x	ne30x8	0.23	9.92	65.13	14.49	1.12
	ne30x8 DIUR	0.26	7.59	54.55	13.53	1.05
	ne30x16	0.32	12.58	73.43	14.93	1.15
	ne30x16 DIUR	0.31	9.63	63.8	13.66	1.06
C ₂ H ₆	ne30x8	0.36	0.39	44.06	9.49	1.38
	ne30x8 DIUR	0.36	0.38	43.04	9.5	1.38
	ne30x16	0.36	0.37	44.62	9.53	1.39
	ne30x16 DIUR	0.38	0.36	43.63	9.53	1.39
C ₃ H ₈	ne30x8	0.27	0.33	67.38	1.65	1.3
	ne30x8 DIUR	0.28	0.33	67.79	1.65	1.3
	ne30x16	0.28	0.46	76.68	1.58	1.25
	ne30x16 DIUR	0.32	0.43	72.08	1.56	1.23
C ₃ H ₆	ne30x8	0.19	0.17	68.82	0.36	1.06
	ne30x8 DIUR	0.21	0.18	68.58	0.35	1.05
	ne30x16	0.19	0.21	77.27	0.36	1.08
	ne30x16 DIUR	0.21	0.2	75.87	0.36	1.07

BENZ	ne30x8	0.21	0.12	58.16	0.17	1.65
	ne30x8 DIUR	0.21	0.12	57.53	0.17	1.64
	ne30x16	0.2	0.15	67.87	0.2	1.94
	ne30x16 DIUR	0.23	0.15	66.83	0.2	1.93
TOLU	ne30x8	0.03	0.51	77.81	0.92	1.46
	ne30x8 DIUR	0.03	0.5	77.59	0.91	1.45
	ne30x16	0.02	0.73	87.91	1.14	1.82
	ne30x16 DIUR	0.03	0.69	82.95	1.11	1.77
ISOP	ne30x8	0.25	0.39	157.91	0.41	4.06
	ne30x8 DIUR	0.29	0.34	148.24	0.35	3.48
	ne30x16	0.4	0.12	133.75	0.12	1.2
	ne30x16 DIUR	0.38	0.12	131.84	0.12	1.23
APIN	ne30x8	0.28	0.03	77.87	0.04	2.33
	ne30x8 DIUR	0.33	0.02	69.02	0.03	1.97
	ne30x16	0.25	0.05	85.88	0.06	3.65
	ne30x16 DIUR	0.32	0.04	76.05	0.06	3.17

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Table S5: Same as Table S4, but for available meteorological parameters.

		CORR	STD	CV	RMSE	NRMSE
RH	ne30x8	0.76	17.99	30.17	13.63	0.73
	ne30x8 DIUR	0.76	18.04	30.17	13.58	0.73
	ne30x16	0.78	17.73	29.92	13.27	0.71
	ne30x16 DIUR	0.78	17.77	29.95	13.2	0.71
H ₂ O	ne30x8	0.89	6501335.69	39.68	3602571.29	0.72
	ne30x8 DIUR	0.89	6430226.01	39.25	3544576.07	0.71
	ne30x16	0.89	6327619.47	38.9	3371758	0.68
	ne30x16 DIUR	0.9	6349449.03	39.1	3355553.72	0.67
WS	ne30x8	0.44	3.04	52.27	4.53	3.87
	ne30x8 DIUR	0.44	2.99	51.07	4.53	3.87
	ne30x16	0.43	2.79	49.56	4.24	3.62
	ne30x16 DIUR	0.43	2.8	49.91	4.23	3.61
WD	ne30x8	0.55	94.09	49.46	78.73	1.46
	ne30x8 DIUR	0.57	93.56	49.64	77.2	1.43
	ne30x16	0.55	92.78	48.91	77.74	1.44
	ne30x16 DIUR	0.55	93.3	49.92	77.96	1.44
PS	ne30x8	0.97	650.84	0.66	234.82	0.4
	ne30x8 DIUR	0.97	651.4	0.66	234.29	0.4
	ne30x16	0.97	652.36	0.66	300.53	0.51
	ne30x16 DIUR	0.97	656.02	0.66	299.16	0.51
T	ne30x8	0.92	5.07	1.72	2.35	0.42
	ne30x8 DIUR	0.92	5.08	1.72	2.34	0.41
	ne30x16	0.93	5.11	1.73	2.23	0.39
	ne30x16 DIUR	0.93	5.08	1.72	2.25	0.4

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Table S6: Detailed statistics for tropospheric NO₂ and HCHO columns from Pandora and four model simulations at the SWDetroitMI site in Southeast Michigan.

		n	CORR	MB	NMB	RMSE	NRMSE
NO2	ne30x8	83	0.27	-7.80E+14	-0.10	4.73E+15	1.18
	ne30x8 DIUR		0.25	-5.69E+14	-0.07	4.58E+15	1.14
	ne30x16		0.28	5.69E+14	0.07	5.07E+15	1.27
	ne30x16 DIUR		0.31	7.31E+14	0.09	4.78E+15	1.19
HCHO	ne30x8	43	0.17	-2.30E+15	-0.22	5.90E+15	1.36
	ne30x8 DIUR		0.30	-2.50E+15	-0.23	5.41E+15	1.25
	ne30x16		0.11	-1.20E+15	-0.11	5.98E+15	1.38
	ne30x16 DIUR		0.22	-1.43E+15	-0.13	5.49E+15	1.27

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Table S7: Detailed statistics for tropospheric NO₂ and HCHO columns from Pandora and four model simulations at the DearbornMI site in Southeast Michigan.

		n	CORR	MB	NMB	RMSE	NRMSE
NO2	ne30x8	160	0.59	-2.89E+13	-0.004	4.16E+15	0.81
	ne30x8 DIUR		0.43	8.10E+14	0.11	4.75E+15	0.92
	ne30x16		0.61	6.50E+14	0.09	4.30E+15	0.83
	ne30x16 DIUR		0.58	1.52E+15	0.21	4.64E+15	0.90
HCHO	ne30x8	113	0.19	-3.01E+15	-0.30	4.94E+15	1.52
	ne30x8 DIUR		0.38	-2.18E+15	-0.22	3.98E+15	1.22
	ne30x16		0.15	-2.50E+15	-0.25	5.33E+15	1.64
	ne30x16 DIUR		0.30	-1.74E+15	-0.17	4.65E+15	1.43

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Table S8: Detailed information of each GCAS raster on flight days during MOOSE 2021.

		Day of Week	Flight Time	Mean Aircraft Altitude (km)	AQI	Temperature	Wind Direction	Wind Speed
	Raster 1 (10 EDT)	Saturday	9:48-11:23 EDT	12.3		23-27°C		6-10 m/s
20210605					108		SW	
	Raster 2 (14 EDT)	Saturday	13:47-15:19 EDT	12.3		28-31°C		6-12 m/s
	Raster 1 (11 EDT)	Friday	10:10-11:45 EDT	12.4		24-28°C		2-4 m/s
20210611	Raster 2 (12 EDT)	Friday	11:45-13:16 EDT	12.4	71	26-29°C	NE	2-4 m/s
	Raster 3 (13 EDT)	Friday	13:16-14:00 EDT	12.4		27-30°C		3-5 m/s
	Raster 1 (10 EDT)	Wednesday	9:16-11:31 EDT	8.7		18-21°C		1-5 m/s
20210616	Raster 2 (13 EDT)	Wednesday	13:05-14:44 EDT	12.1	51	20-24°C	N	3-8 m/s
	Raster 3 (15 EDT)	Wednesday	14:44-16:15 EDT	12.2		20-24°C		2-8 m/s
20210617	Raster 1 (10 EDT)	Thursday	9:18-10:56 EDT	12.3	100	17-21°C	SW	3-6 m/s

	Raster 2 (11 EDT)	Thursday	10:56-12:29 EDT	12.3		22-25°C		4-7 m/s
	Raster 3 (15 EDT)	Thursday	14:10-15:44 EDT	12.3		26-28°C		4-12 m/s
	Raster 1 (9 EDT)	Tuesday	8:51-10:40 EDT	12		11-13°C		2-7 m/s
20210622	Raster 2 (11 EDT)	Tuesday	10:40-12:24 EDT	12	27	15-16°C	NE	3-7 m/s
	Raster 3 (13 EDT)	Tuesday	12:25-14:44 EDT	11.2		16-17°C		2-6 m/s
	Raster 1 (9 EDT)	Thursday	8:31-10:23 EDT	10.8		21-23°C		6-14 m/s
20210624					77		S	
	Raster 2 (11 EDT)	Thursday	10:23-12:24 EDT	9		22-24°C		8-16 m/s

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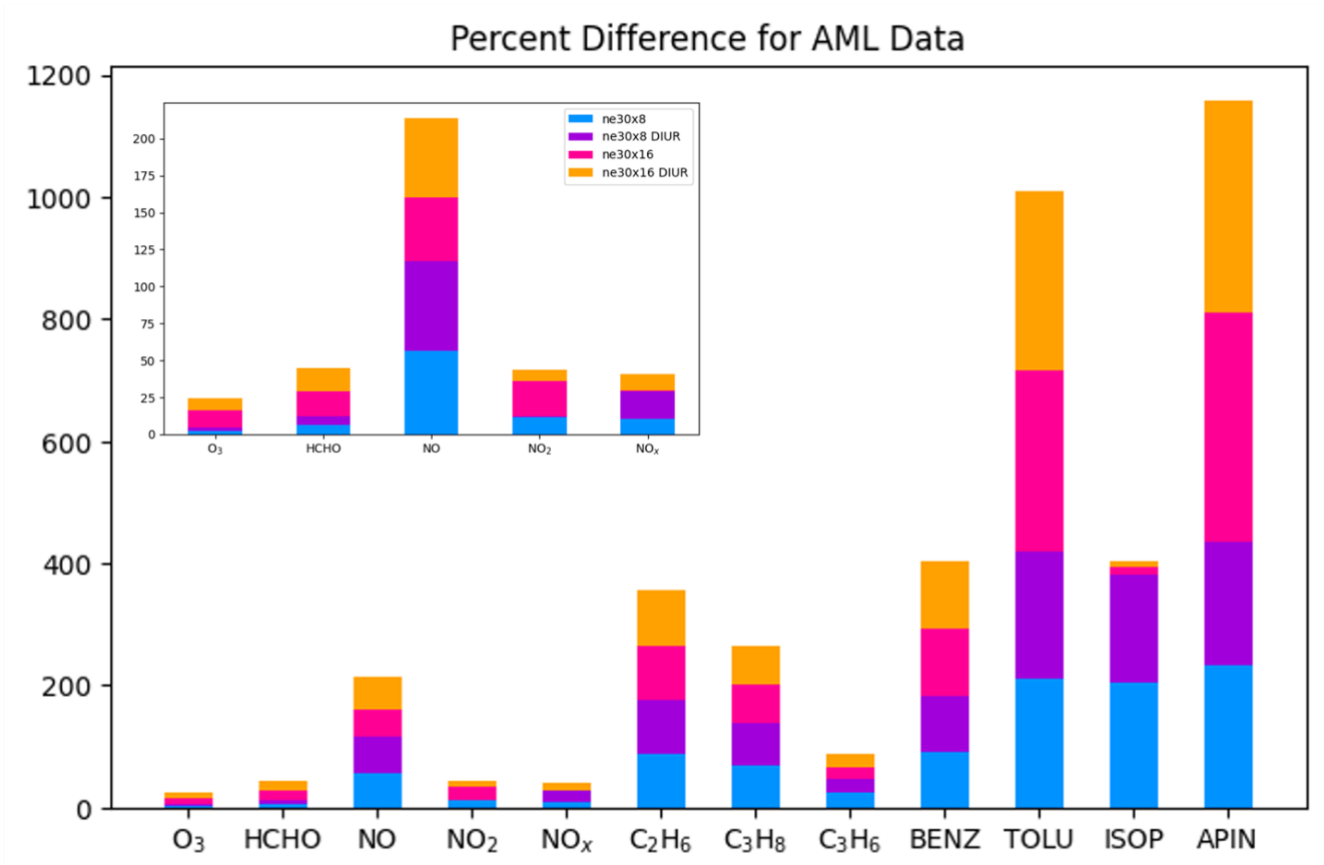


Figure S1: Percent differences between the Aerodyne Mobile Laboratory (AML) observations and MUSICAv0 model simulations used in this study.

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NO₂ Tropospheric Column [20210605 R1]

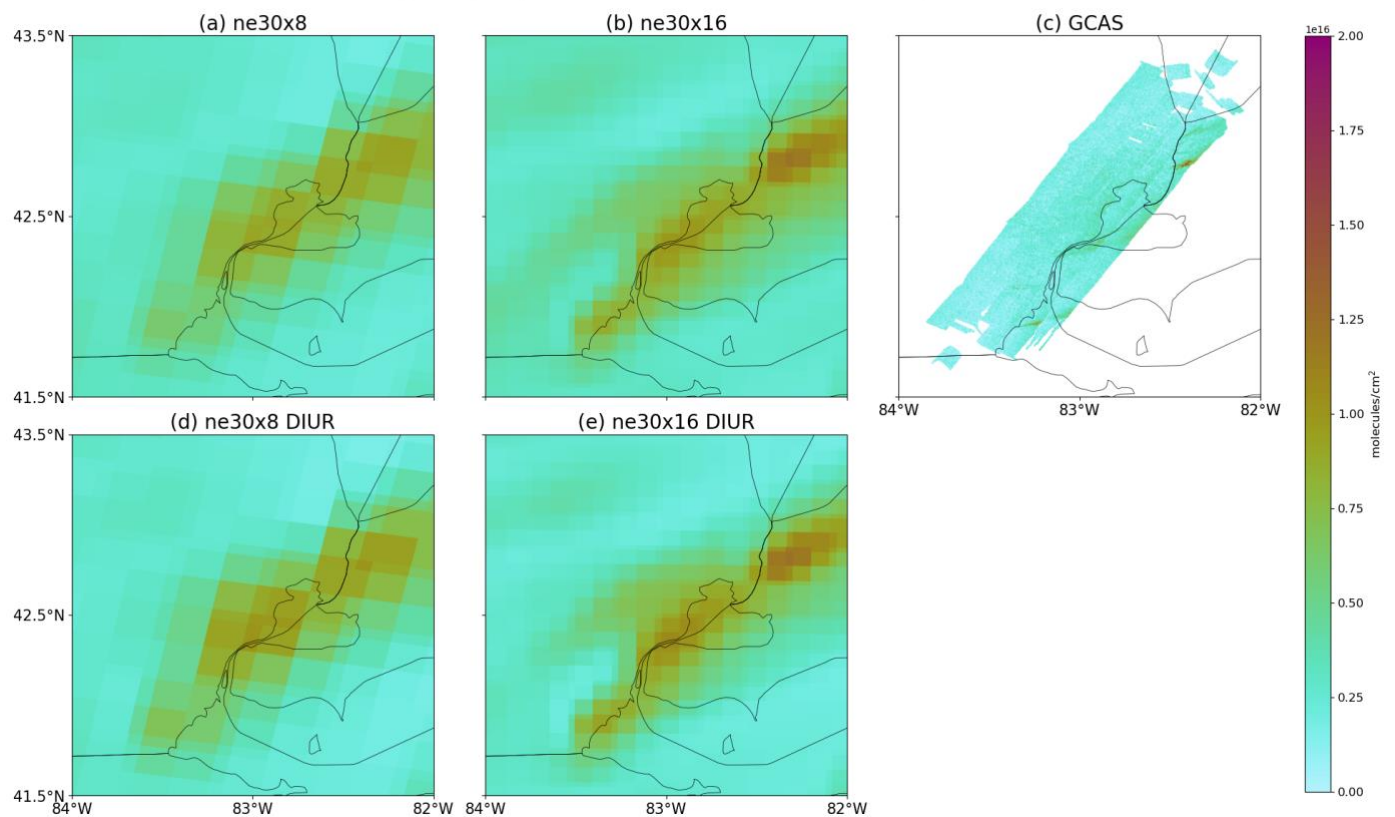


Figure S2: Modeled and observed NO₂ tropospheric columns over Southeast Michigan on 5 June 2021. The GCAS instrument flew over the Southeast Michigan region between 9:48 and 11:23 EDT, so modeled NO₂ tropospheric columns were calculated using the 11 EDT time frame. Figures S2a, S2b, S2d, and S2e represent modeled NO₂ tropospheric columns calculated to about 12 km in altitude, which was the average flight altitude of the NASA Gulfstream-III aircraft. Figure S2c shows observed NO₂ tropospheric columns from the GCAS instrument during the morning time.

NO₂ Tropospheric Column [20210605 R2]

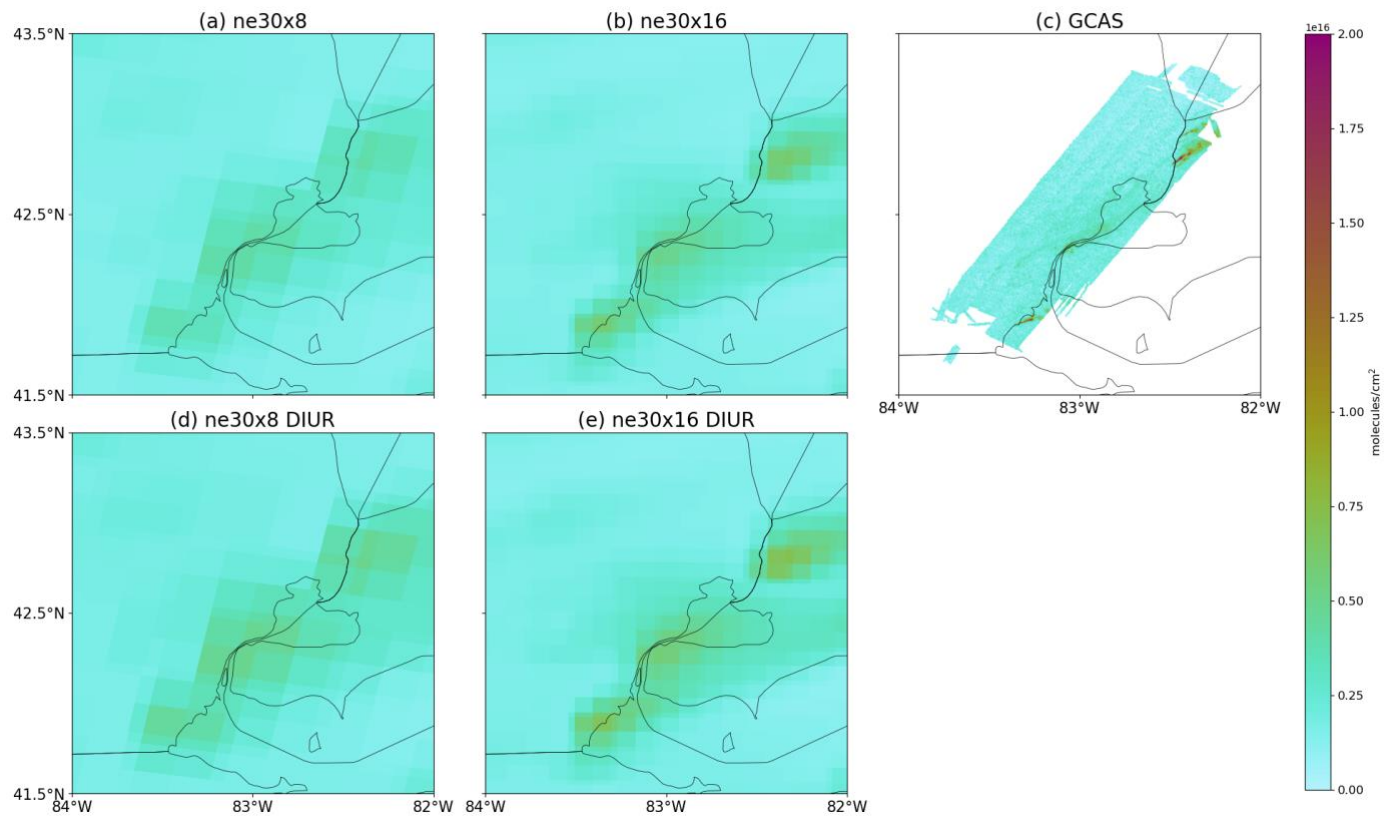


Figure S3: Same as Fig. S2, but the GCAS instrument flew over Southeast Michigan from 13:47 to 15:19 EDT, and modeled NO₂ tropospheric columns were calculated during the 14 EDT time frame.

NO₂ Tropospheric Column [20210616 R1]

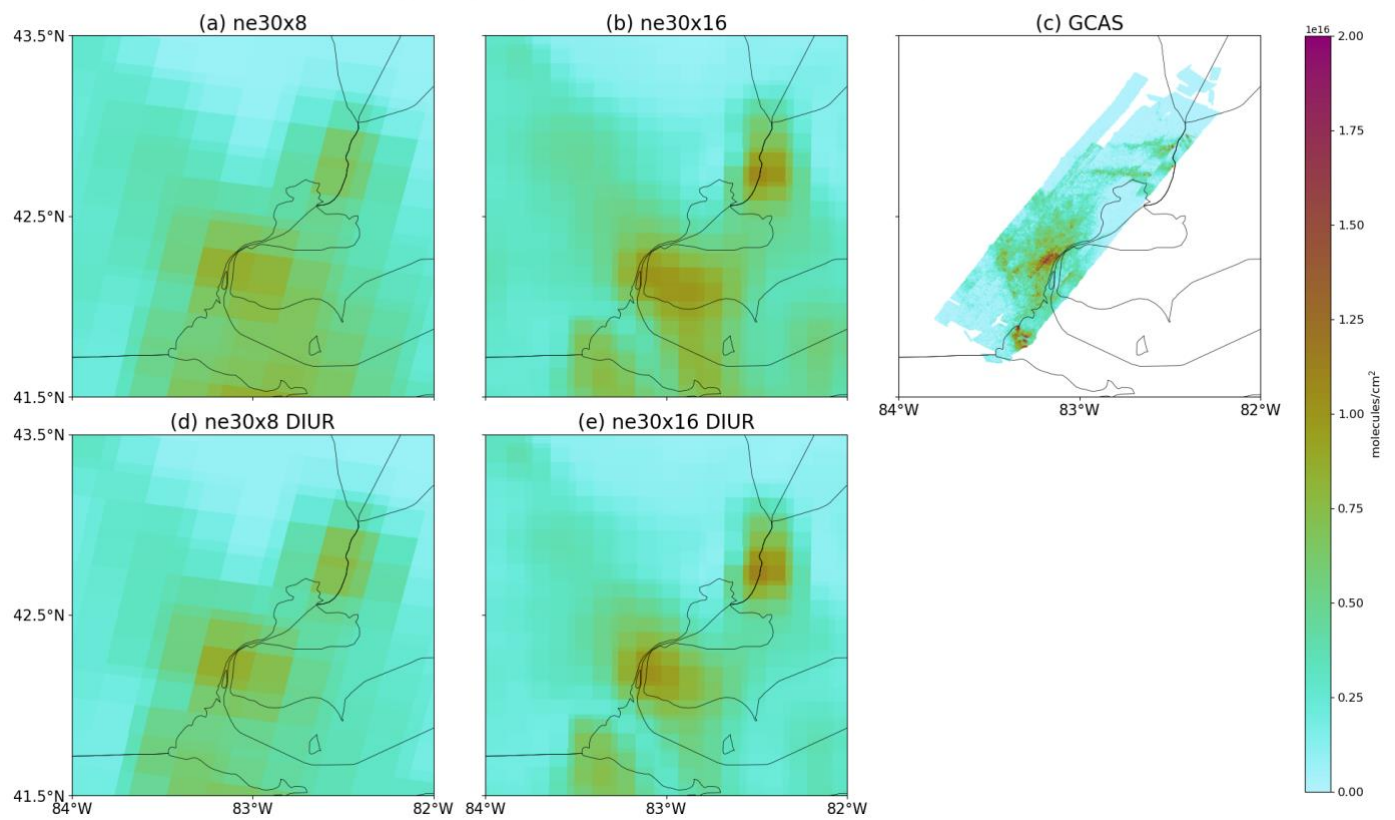


Figure S4: Modeled and observed NO₂ tropospheric columns over Southeast Michigan on 16 June 2021. The GCAS instrument flew over the Southeast Michigan region between 9:16 and 11:31 EDT, so modeled NO₂ tropospheric columns were calculated using the 10 EDT time frame. Figures S4a, S4b, S4d, and S4e represent modeled NO₂ tropospheric columns calculated to about 12 km in altitude, which was the average flight altitude of the NASA Gulfstream-III aircraft. Figure S4c shows observed NO₂ tropospheric columns from the GCAS instrument during the morning time.

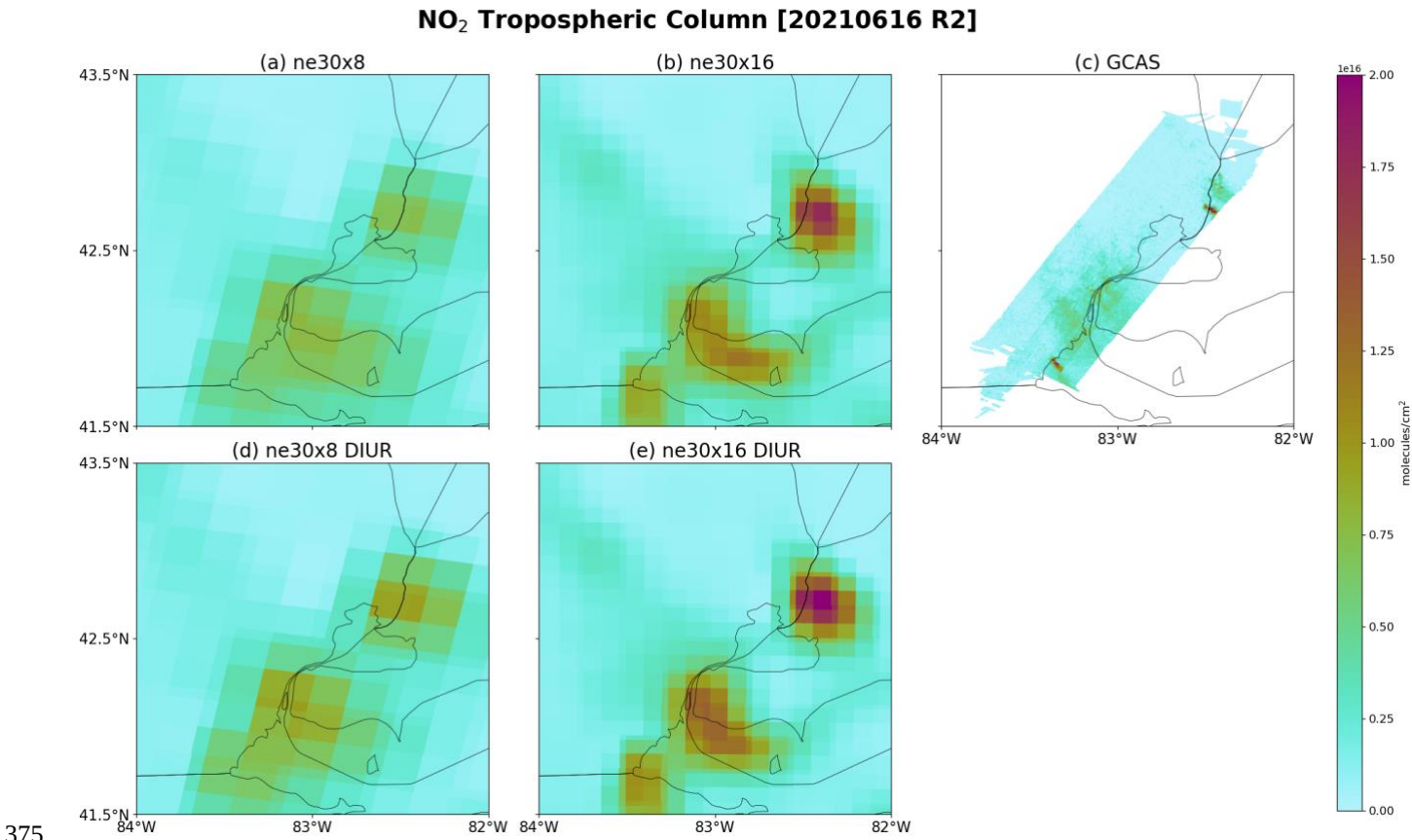


Figure S5: Same as Fig. S4, but the GCAS instrument flew over Southeast Michigan from 13:05 to 14:44 EDT, and modeled NO₂ tropospheric columns were calculated during the 13 EDT time frame.

NO₂ Tropospheric Column [20210616 R3]

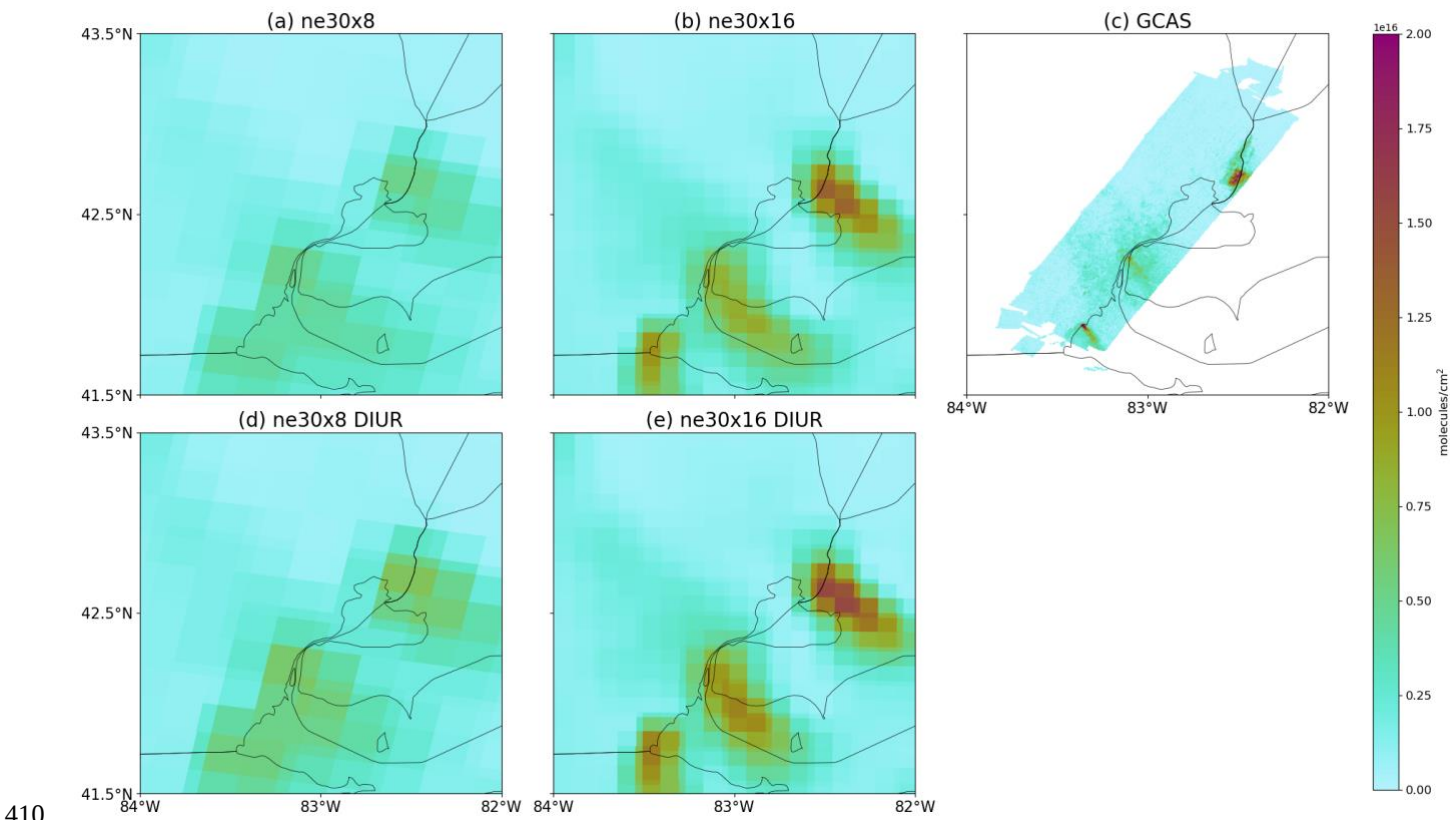


Figure S6: Same as Fig. S4, but the GCAS instrument flew over Southeast Michigan from 14:44 to 16:15 EDT, and modeled NO₂ tropospheric columns were calculated during the 15 EDT time frame.

NO₂ Tropospheric Column [20210617 R1]

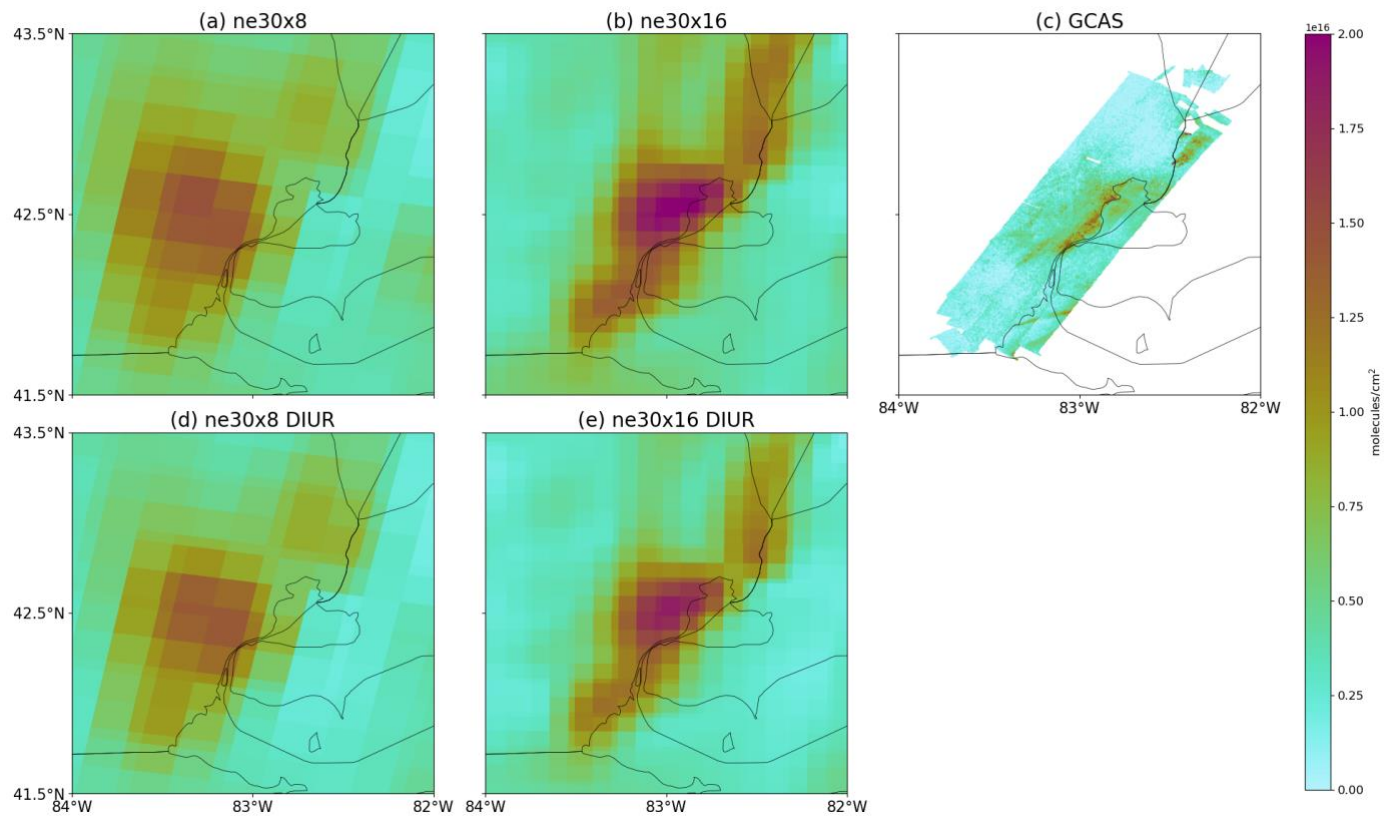


Figure S7: Modeled and observed NO₂ tropospheric columns over Southeast Michigan on 17 June 2021. The GCAS instrument flew over the Southeast Michigan region between 9:18 and 10:56 EDT, so modeled NO₂ tropospheric columns were calculated using the 10 EDT time frame. Figures S7a, S7b, S7d, and S7e represent modeled NO₂ tropospheric columns calculated to about 12 km in altitude, which was the average flight altitude of the NASA Gulfstream-III aircraft. Figure S7c shows observed NO₂ tropospheric columns from the GCAS instrument during the morning time.

NO₂ Tropospheric Column [20210617 R2]

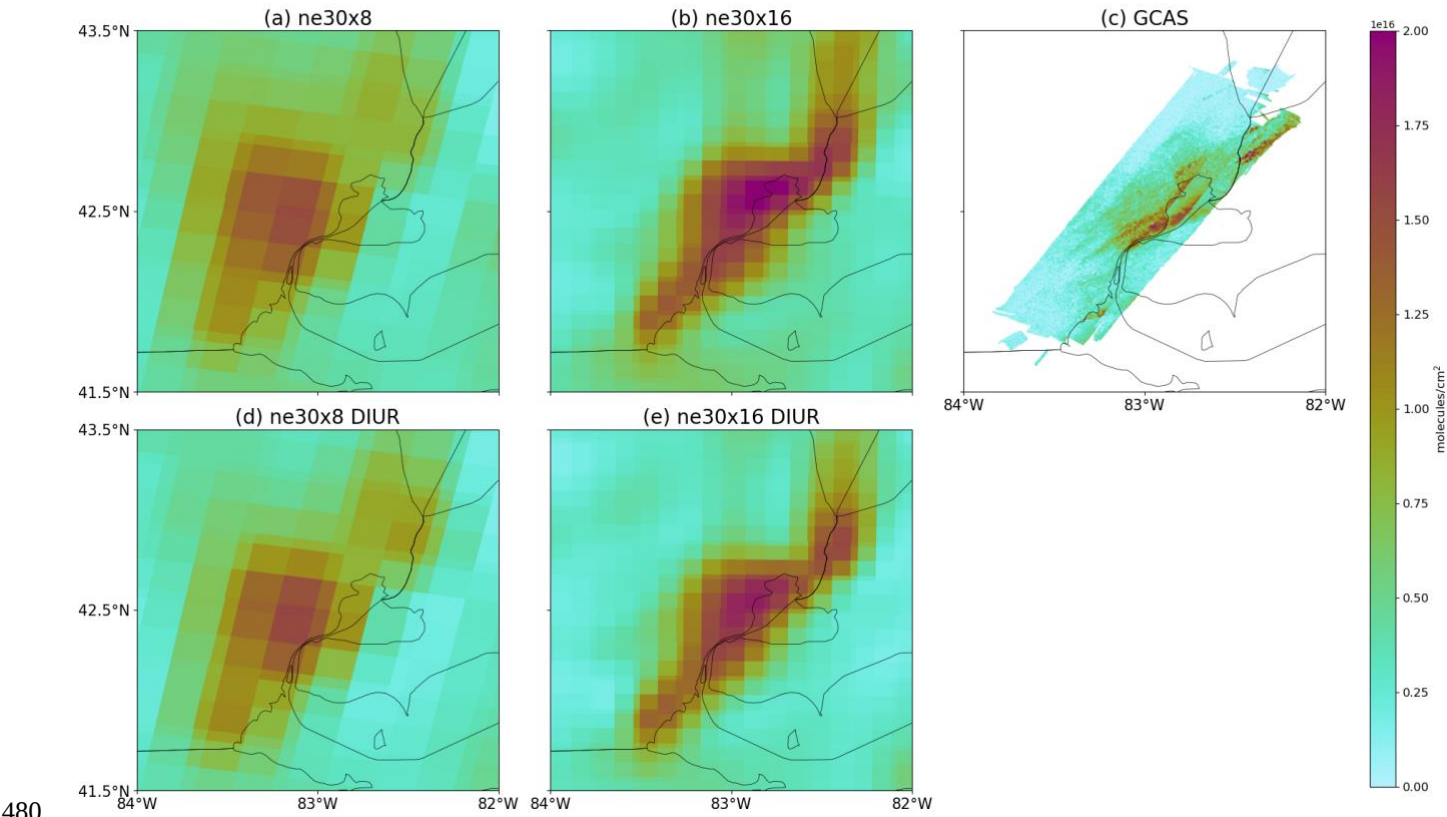


Figure S8: Same as Fig. S7, but the GCAS instrument flew over Southeast Michigan from 10:56 to 12:29 EDT, and modeled NO₂ tropospheric columns were calculated during the 11 EDT time frame.

NO₂ Tropospheric Column [20210617 R3]

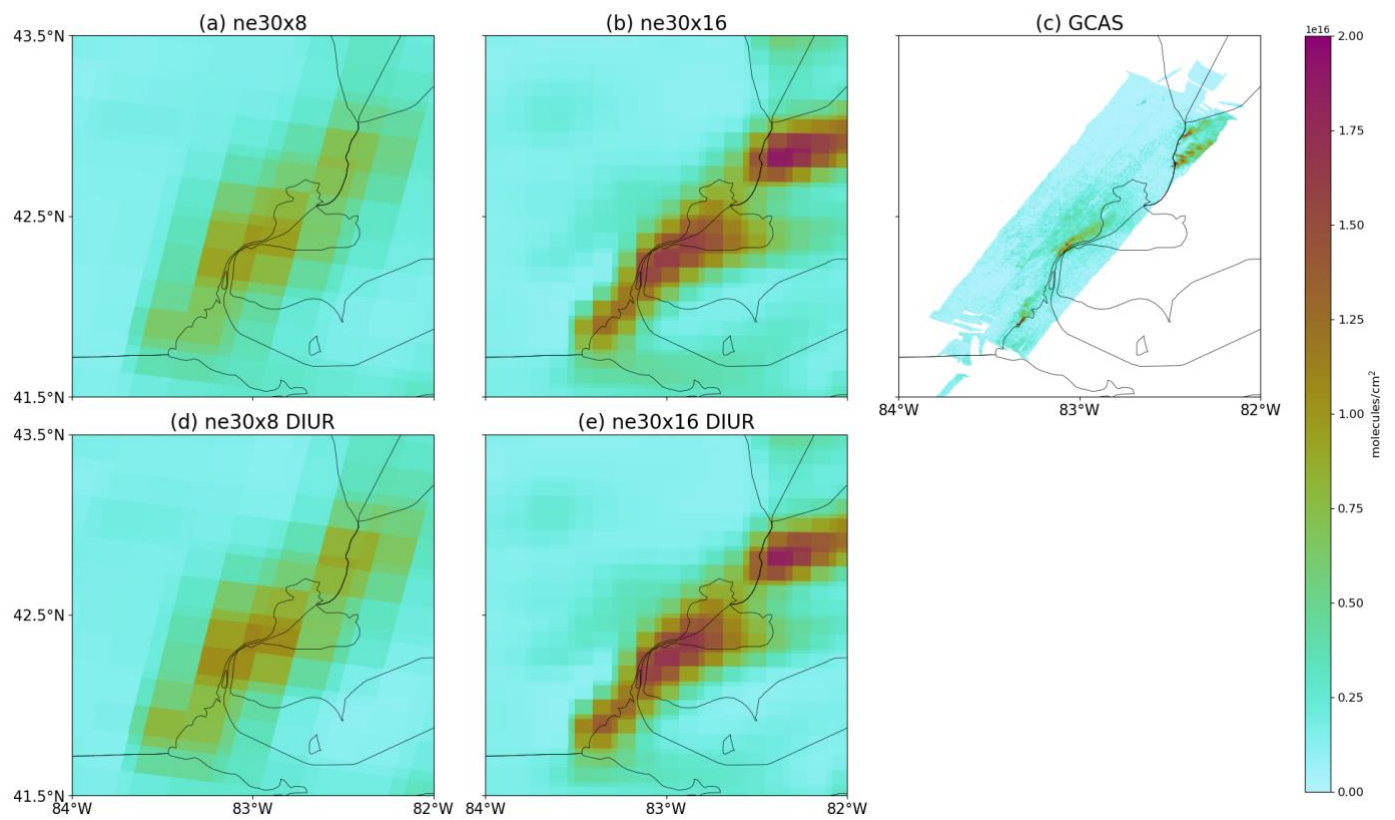


Figure S9: Same as Fig. S7, but the GCAS instrument flew over Southeast Michigan from 14:10 to 15:44 EDT, and modeled NO₂ tropospheric columns were calculated during the 15 EDT time frame.

NO₂ Tropospheric Column [20210622 R1]

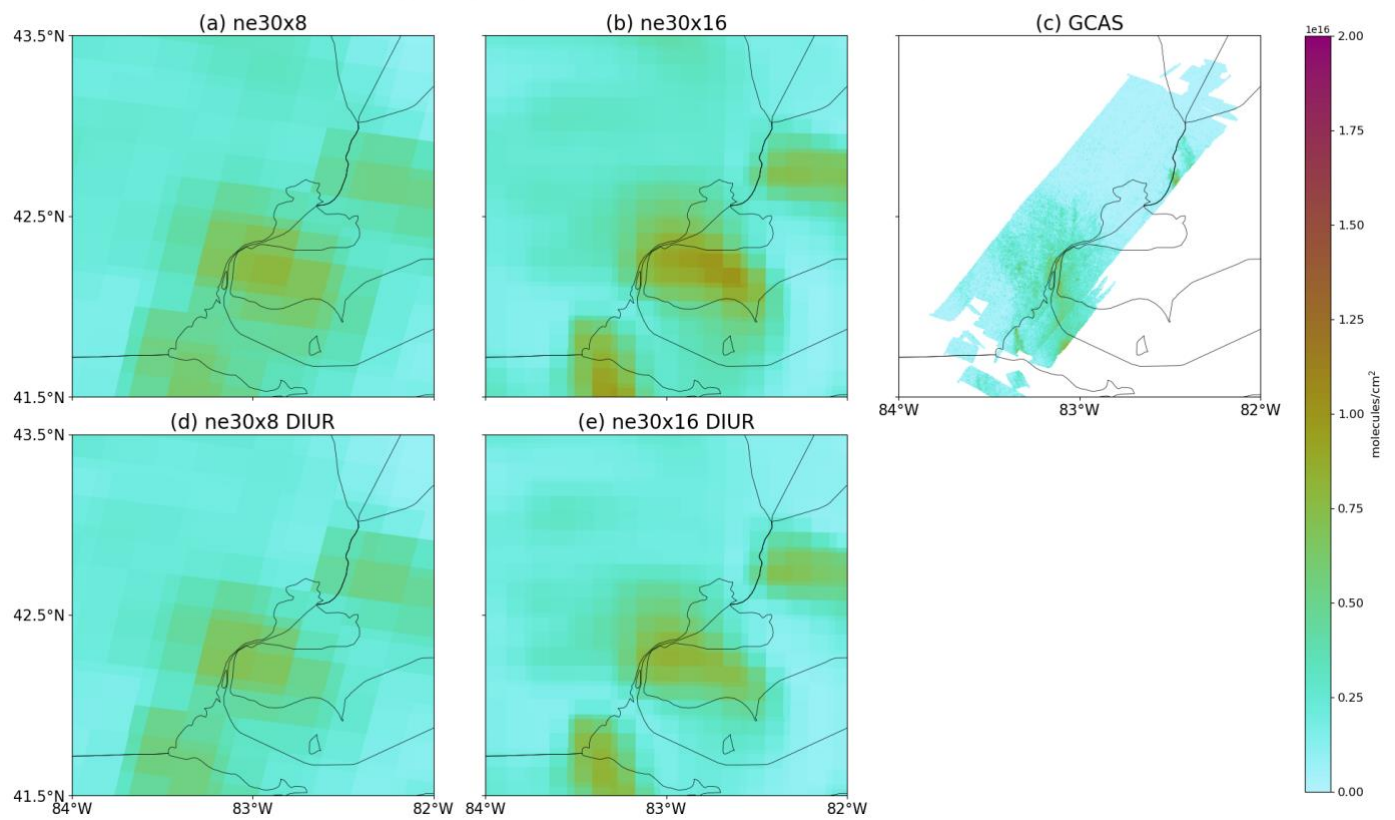


Figure S10: Modeled and observed NO₂ tropospheric columns over Southeast Michigan on 22 June 2021. The GCAS instrument flew over the Southeast Michigan region between 8:51 and 10:41 EDT, so modeled NO₂ tropospheric columns were calculated using the 9 EDT time frame. Figures S10a, S10b, S10d, and S10e represent modeled NO₂ tropospheric columns calculated to about 12 km in altitude, which was the average flight altitude of the NASA Gulfstream-III aircraft. Figure S10c shows observed NO₂ tropospheric columns from the GCAS instrument during the morning time.

NO₂ Tropospheric Column [20210622 R2]

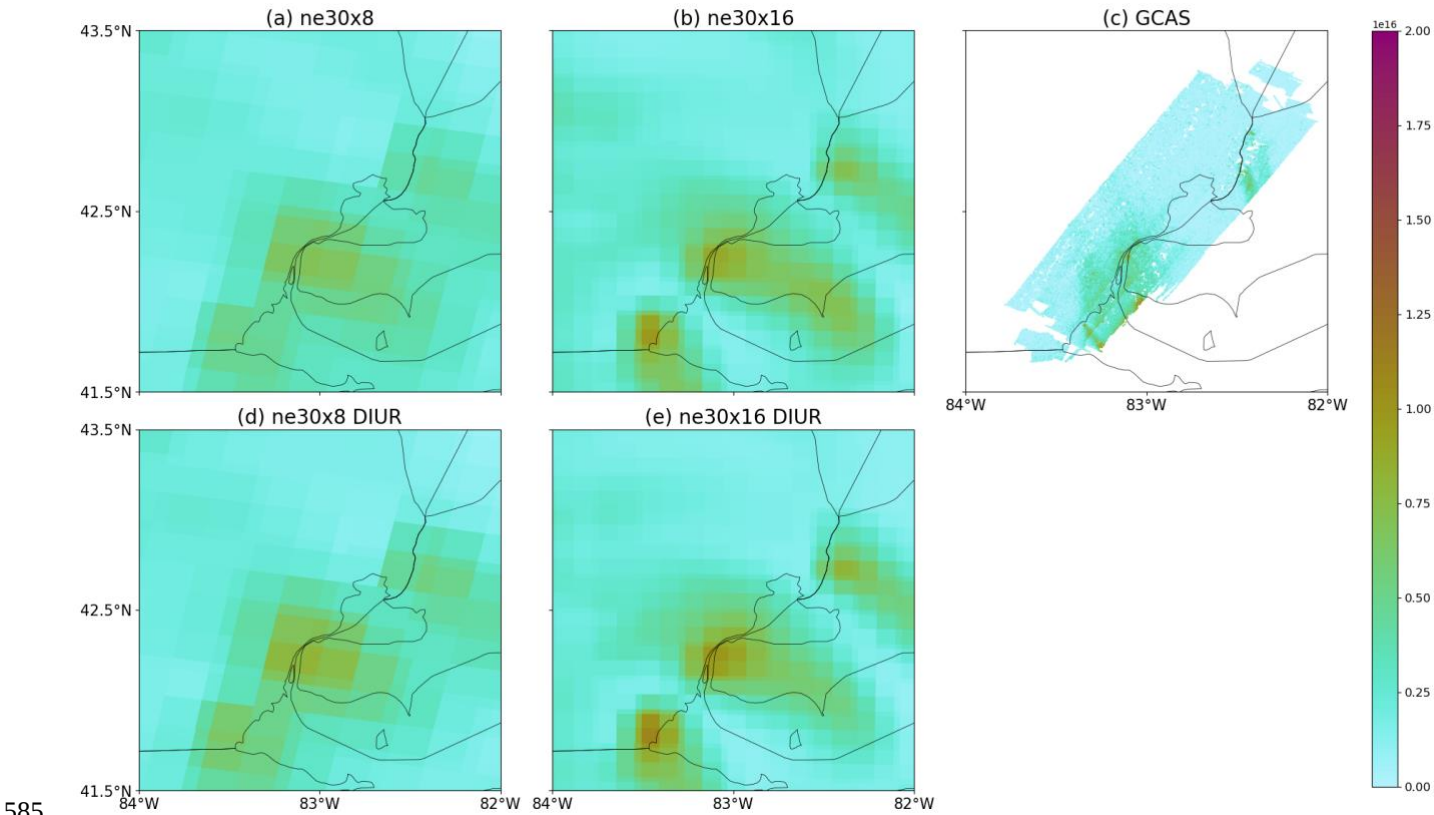


Figure S11: Same as Fig. S10, but the GCAS instrument flew over Southeast Michigan from 10:40 to 12:24 EDT, and modeled NO₂ tropospheric columns were calculated during the 11 EDT time frame.

NO₂ Tropospheric Column [20210622 R3]

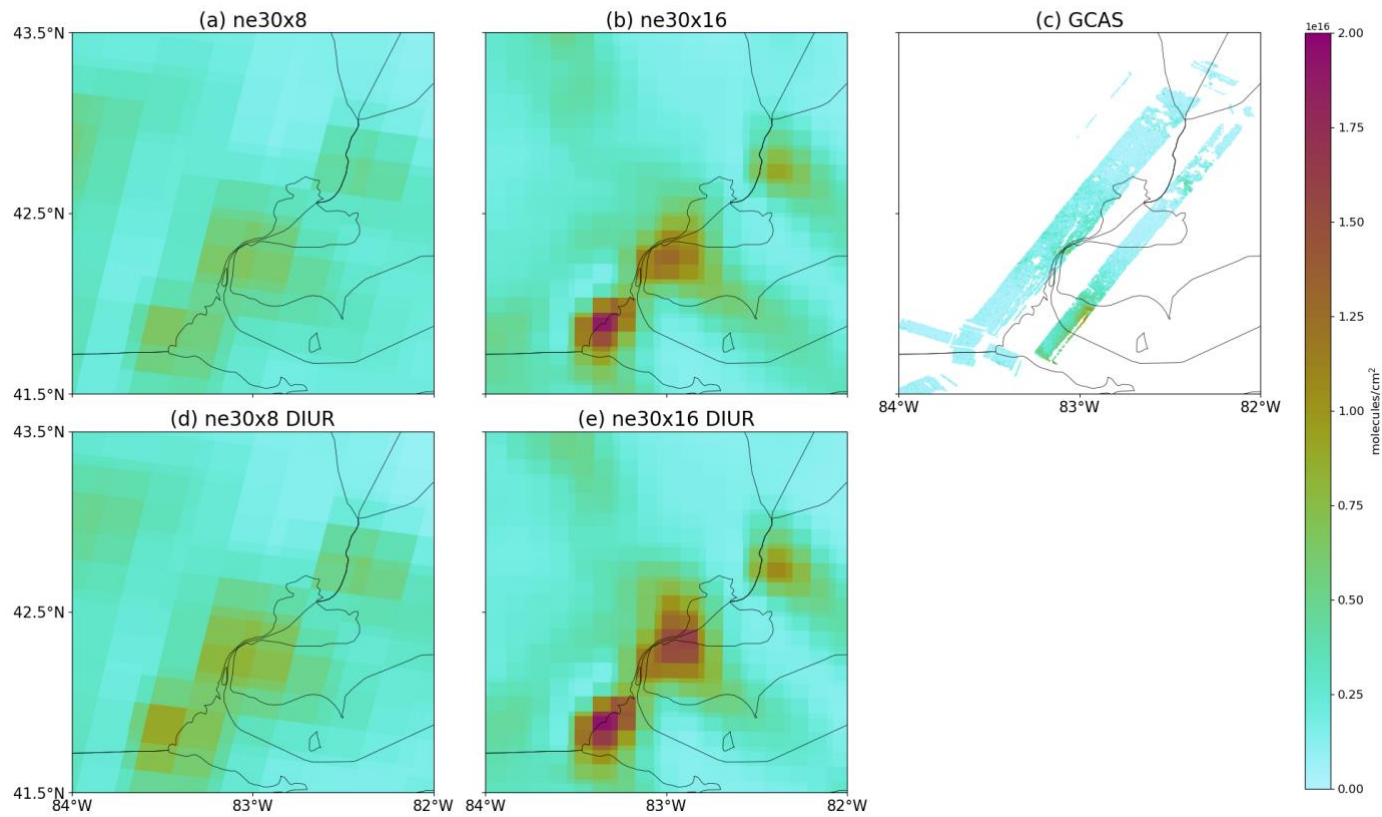


Figure S12: Same as Fig. S10, but the GCAS instrument flew over Southeast Michigan from 12:25 to 14:44 EDT, and modeled NO₂ tropospheric columns were calculated during the 13 EDT time frame.

NO₂ Tropospheric Column [20210624 R1]

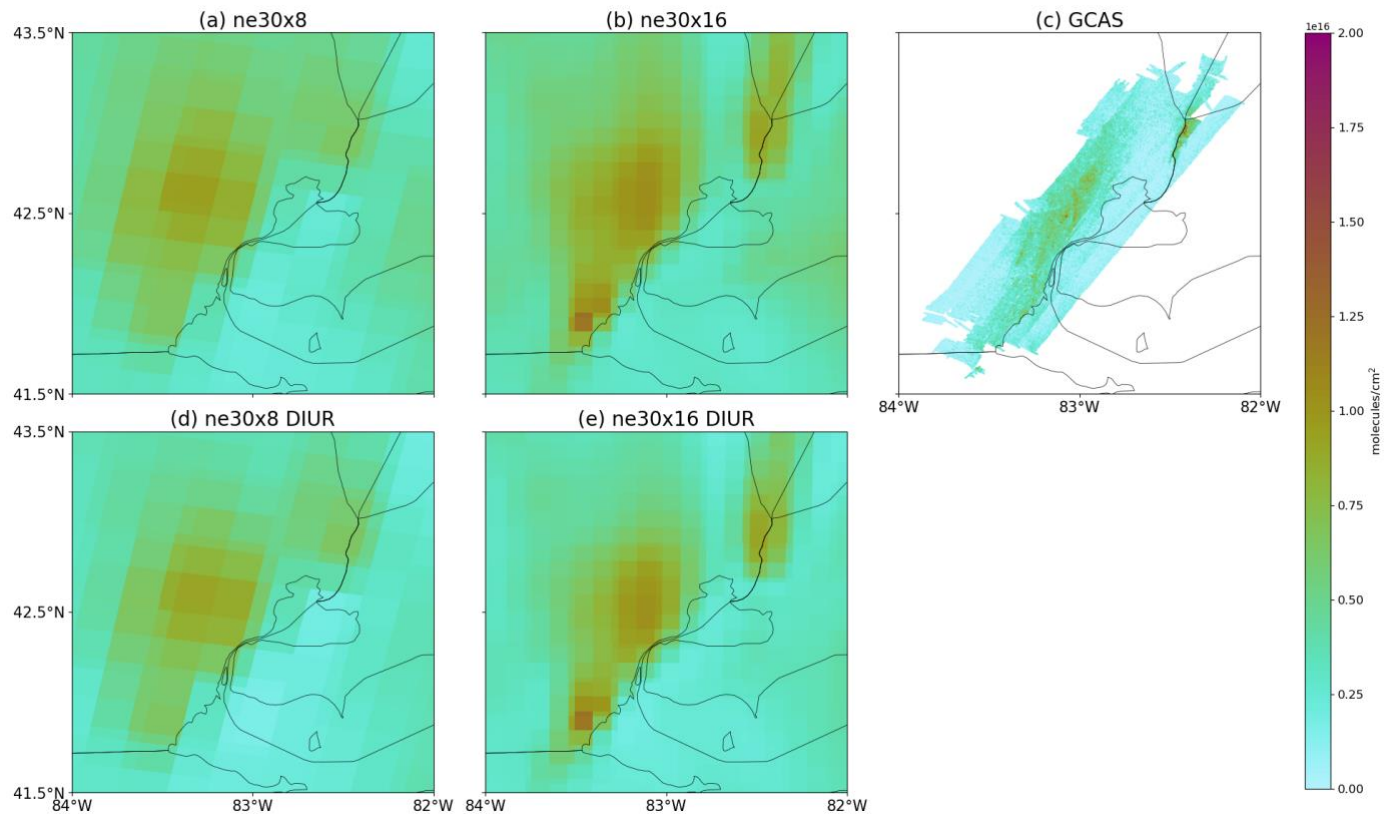


Figure S13: Modeled and observed NO₂ tropospheric columns over Southeast Michigan on 24 June 2021. The GCAS instrument flew over the Southeast Michigan region between 8:31 and 10:23 EDT, so modeled NO₂ tropospheric columns were calculated using the 9 EDT time frame. Figures S13a, S13b, S13d, and S13e represent modeled NO₂ tropospheric columns calculated to about 12 km in altitude, which was the average flight altitude of the NASA Gulfstream-III aircraft. Figure S13c shows observed NO₂ tropospheric column from the GCAS instrument during the morning time.

NO₂ Tropospheric Column [20210624 R2]

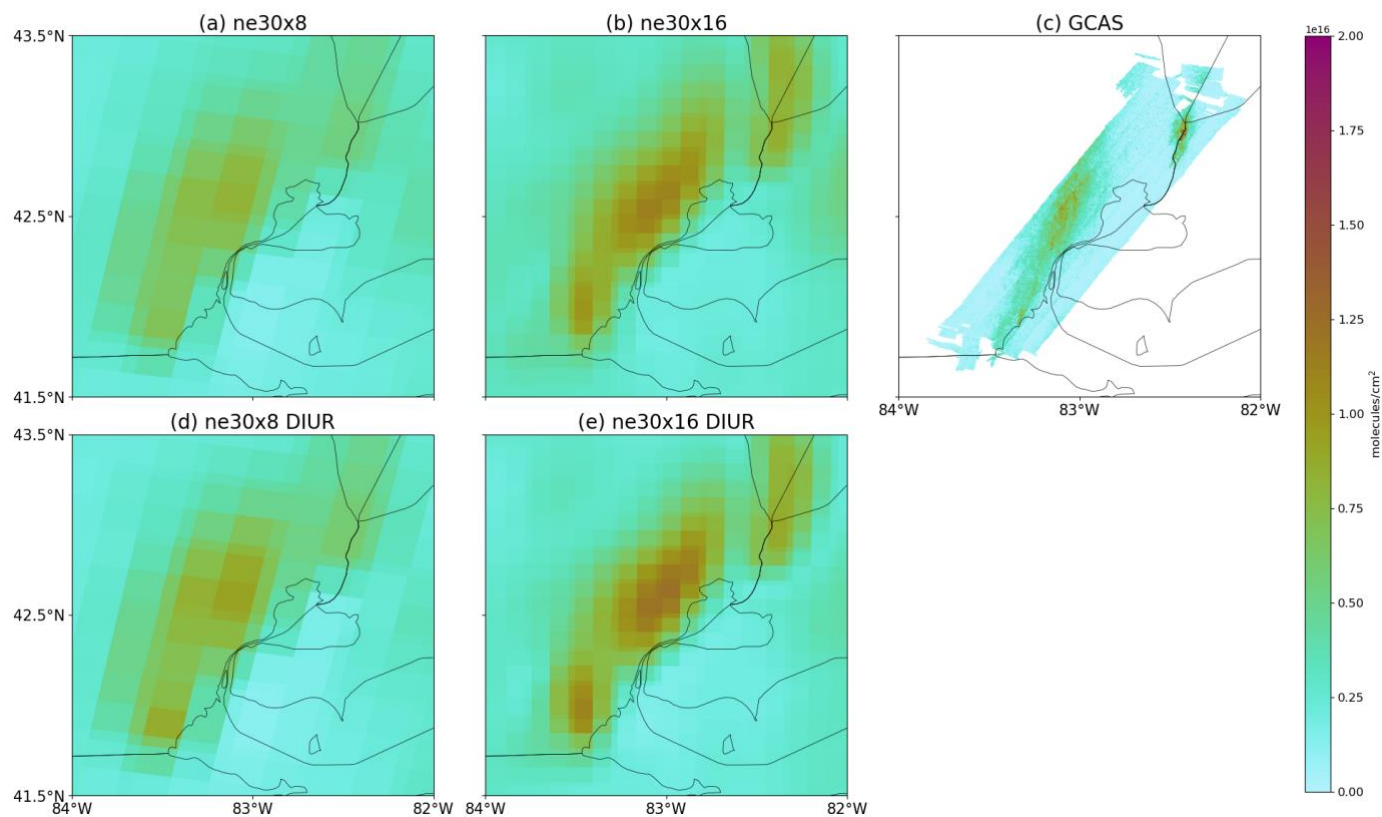


Figure S14: Same as Fig. S13, but the GCAS instrument flew over Southeast Michigan from 10:23 to 12:24 EDT, and modeled NO₂ tropospheric columns were calculated during the 11 EDT time frame.