Supplement of

An intercomparison of satellite, airborne, and ground-level observations with WRF-CAMx simulations of NO_2 columns over Houston, TX during the September 2021 TRACER-AQ campaign

Nawaz et al.

Correspondence to M. Omar Nawaz (nawaz.muhammad@email.gwu.edu)

Table S1: WRF physics options and data sources

WRF Option	Option Selected
Analysis Data	0.25° GDAS (IC/BCs and analysis nudging on the 36 and 12 km domains)
Microphysics	Thompson
Longwave Radiation	Rapid Radiative Transfer Model (RRTMG)
Shortwave Radiation	RRTMG
Surface Layer Physics	Revised MM5 surface layer scheme
LSM	Noah
PBL scheme	Yonsei University (YSU)
Cumulus scheme	Multi-Scale Kain-Fritsch (MSKF) on 36/12 km; none for 4/1.333/0.444 km

Table S2: Vertical layer mapping from WRF to CAMx

WRF Layer No.	WRF Eta Level	WRF Layer Pressure (mb)	WRF Layer Top (m)	CAMx Layer No.	CAMx Layer Top (m)	CAMx Layer Thickness (m)
44	0.000	50.00	20576			
43	0.010	59.63	19458			
42	0.025	74.08	18082	30	18082	3885
41	0.045	93.35	16616			
40	0.065	112.61	15427			
39	0.090	136.69	14198	29	14198	2977
38	0.115	160.77	13169			
37	0.145	189.67	12120			
36	0.175	218.57	11221	28	11221	1850
35	0.210	252.28	10304			
34	0.250	290.81	9372	27	9372	1599
33	0.290	329.34	8534			
32	0.330	367.87	7773	26	7773	1269
31	0.370	406.40	7073			
30	0.405	440.12	6504	25	6504	1040
29	0.440	473.83	5969			
28	0.475	507.54	5464	24	5464	870
27	0.510	541.26	4985			
26	0.540	570.16	4594	23	4594	737
25	0.570	599.05	4219			
24	0.600	627.95	3857	22	3857	684
23	0.630	656.85	3509			
22	0.660	685.75	3174	21	3174	325
21	0.690	714.64	2849	20	2849	314
20	0.720	743.54	2535	19	2535	304
19	0.750	772.44	2231	18	2231	247
18	0.775	796.52	1984	17	1984	241
17	0.800	820.60	1744	16	1744	235
16	0.825	844.68	1509	15	1509	230
15	0.850	868.76	1279	14	1279	135
14	0.865	883.21	1144	13	1144	134
13	0.880	897.66	1010	12	1010	132
12	0.895	912.11	878	11	878	130
11	0.910	926.56	748	10	748	86
10	0.920	936.19	662	9	662	85
9	0.930	945.82	577	8	577	84

8	0.940	955.46	493	7	493	84
7	0.950	965.09	409	6	409	83
6	0.960	974.72	326	5	326	82
5	0.970	984.35	243	4	243	82
4	0.980	993.99	162	3	162	81
3	0.990	1003.62	81	2	81	48
2	0.996	1009.40	32	1	32	32
1	0.998	1011.32	16			
surface	1.000	1013.25	0	0	0	

Table S3: Science options for the CAMx simulation

Science Options	CAMx Configuration
Version	Version 7.20
Time Zone	CST
Vertical Grid Mesh	30 Layers with 32 m deep surface layer and 15 layers in the lowest 1.5 km
Horizontal Grids	2-way nested grids with spacings of 1.333 and 0.444 km
Meteorology	2021 WRF meteorology
Chemistry Mechanism	CB6r5 gas-phase mechanism
Chemistry Solver	EBI
Probing Tool	Ozone Source Apportionment Technology (OSAT)
Photolysis Rates	TUV version 4.8 with TOMS ozone column adjustment and in-line adjustment for clouds
Advection Scheme	Piecewise Parabolic Method (PPM)
Planetary Boundary Layer (PBL) mixing	K-theory with KV100 patch to enhance vertical mixing over urban areas within the lowest 100 m
In-line Ix Emissions On	Inorganic iodine (Ix) emissions from saltwater areas
Parallelization	MPI (18 threads) and OMP (6 threads)

Table S4: Major energy generation units in and around Houston, TX and their monthly NOx emissions

Number	Energy Generation Unit	NOx (tons/month)
1	Air Liquide Bayport Complex	570.7
2	Cedar Bayou	73.0
3	W A Parish	34.7
4	Odyssey Energy Altura Cogen, LLC	34.6
5	Texas City Cogeneration	30.8
6	Pasadena Power Plant	27.4
7	Channelview Cogeneration Facility	25.9
8	Deer Park Energy Center	25.0
9	South Houston Green Power Site	25.0
10	TH Wharton	18.1
11	Greens Bayou	11.6

Figure S1: Ratio of TROPOMI NO_2 columns with the new CAMx AMF compared to the operational AMF.

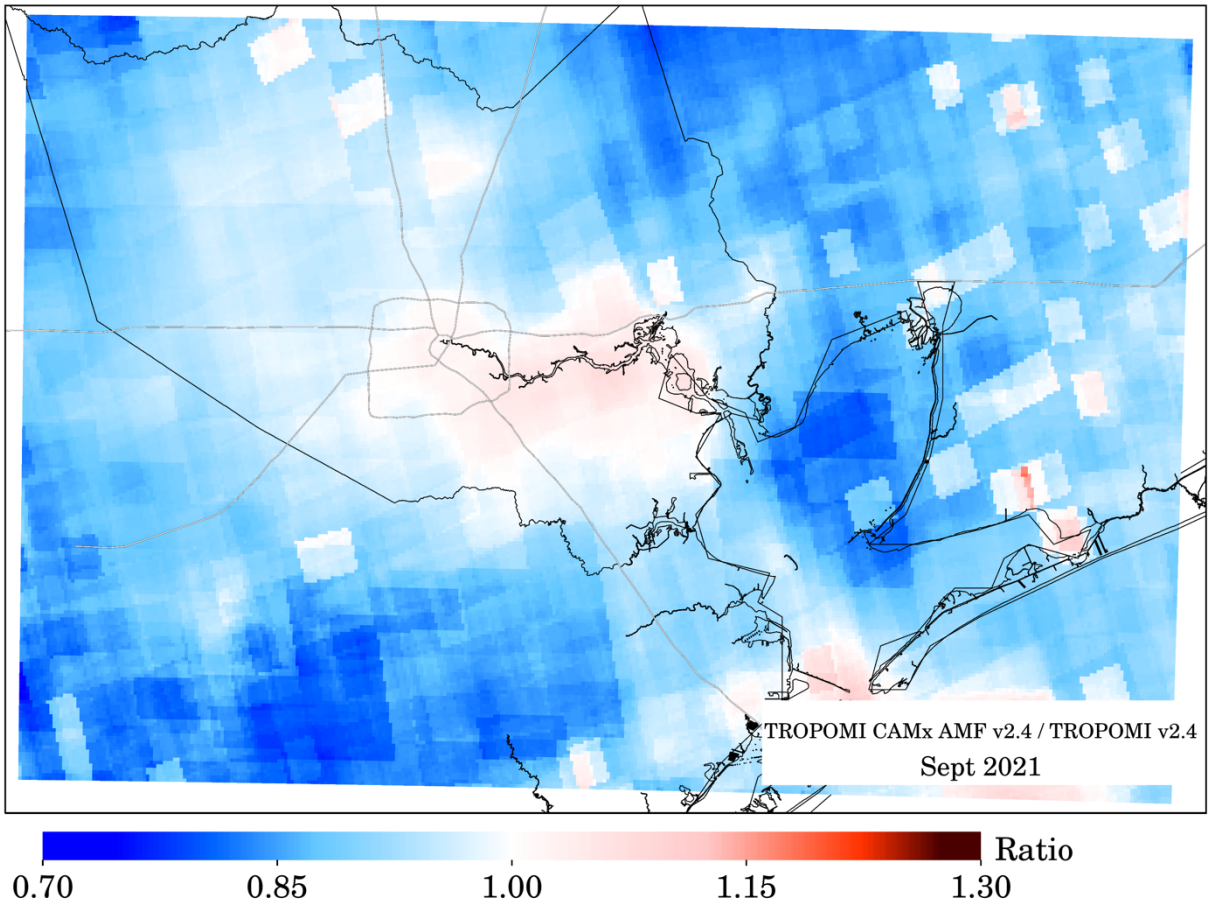

Figure S2: Spatial comparison of GCAS, TROPOMI, and CAMx on September 1, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

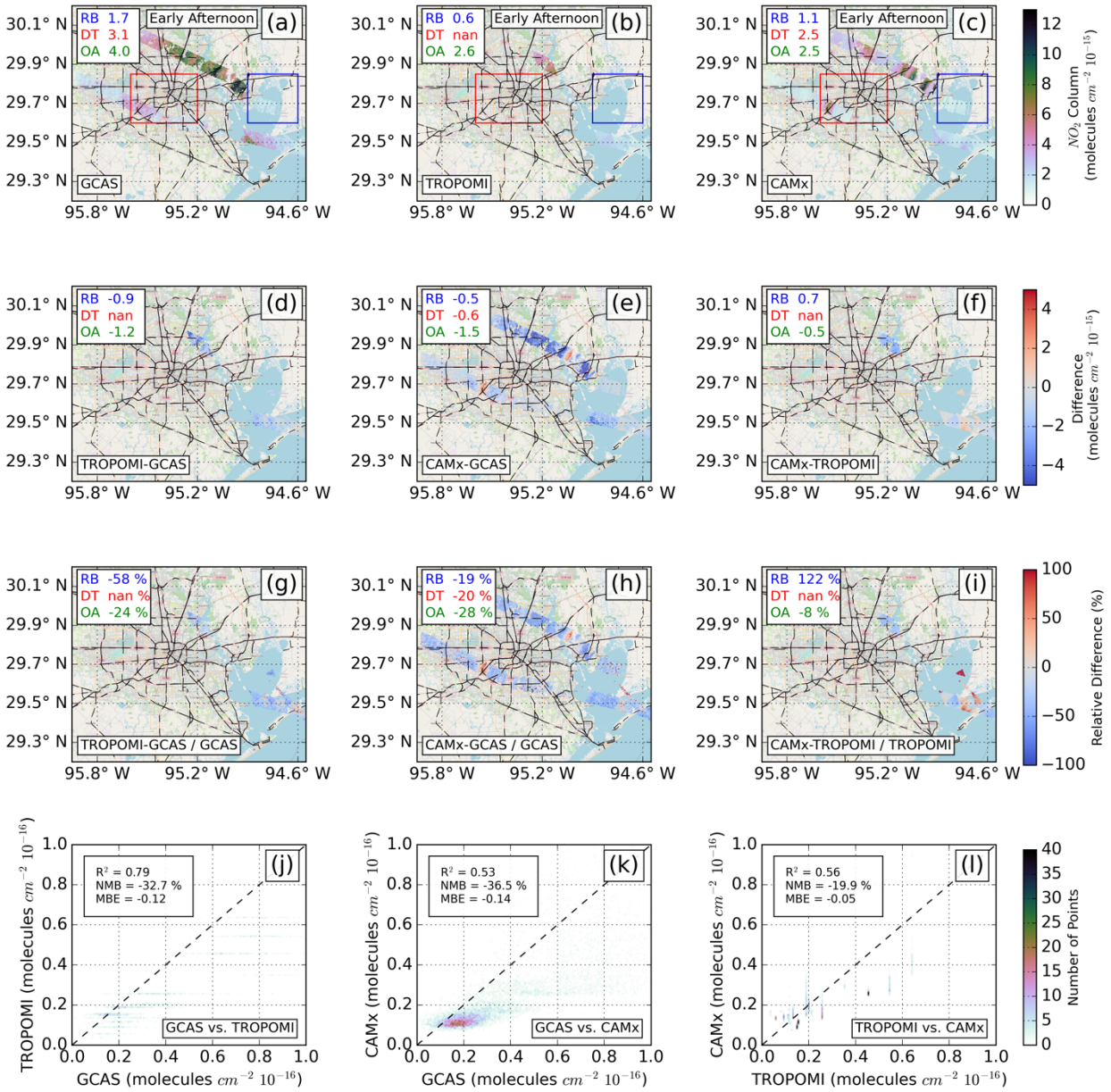

Figure S3: Spatial comparison of GCAS, TROPOMI, and CAMx on September 3, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

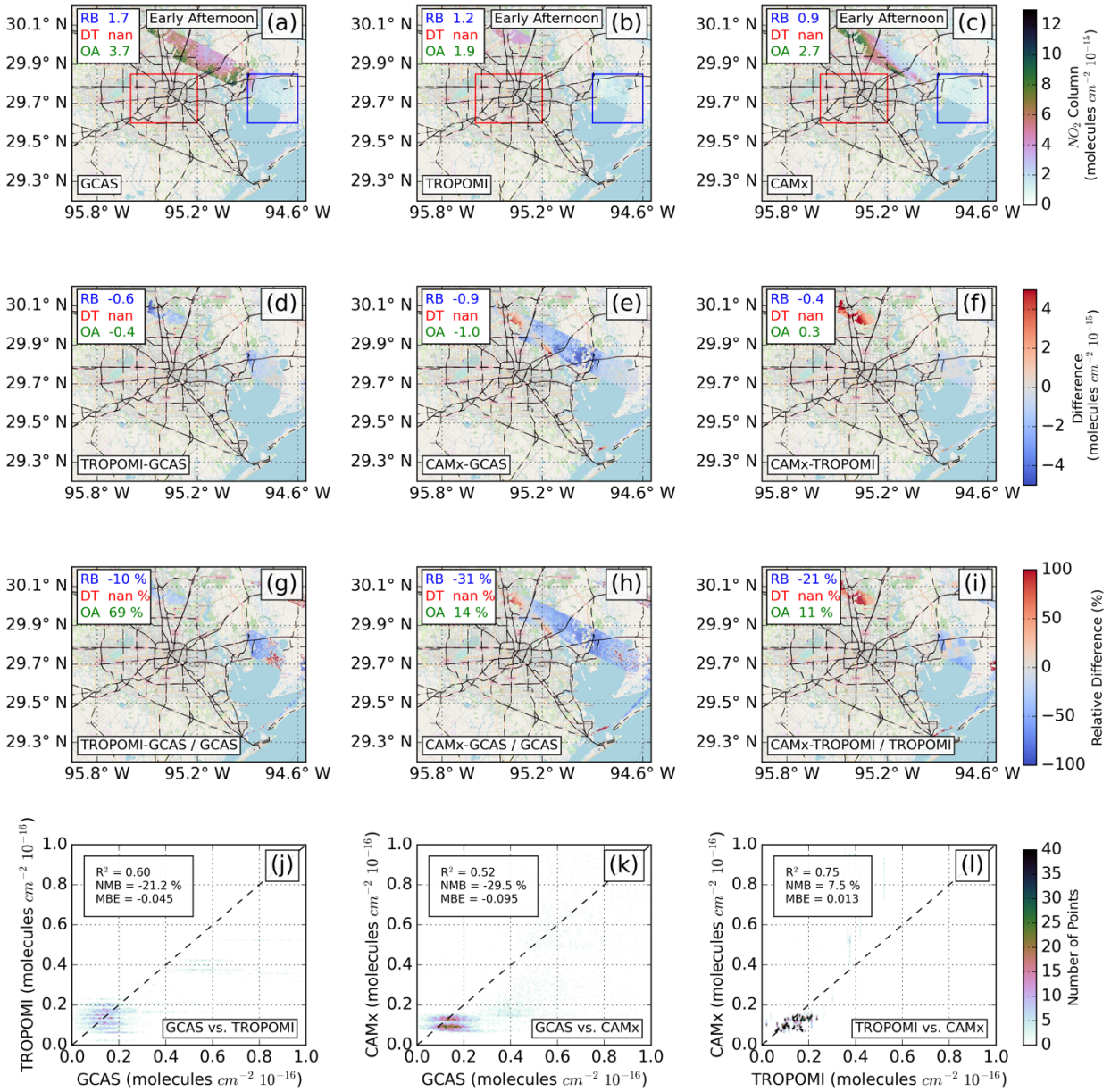

Figure S4: Spatial comparison of GCAS, TROPOMI, and CAMx on September 8, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

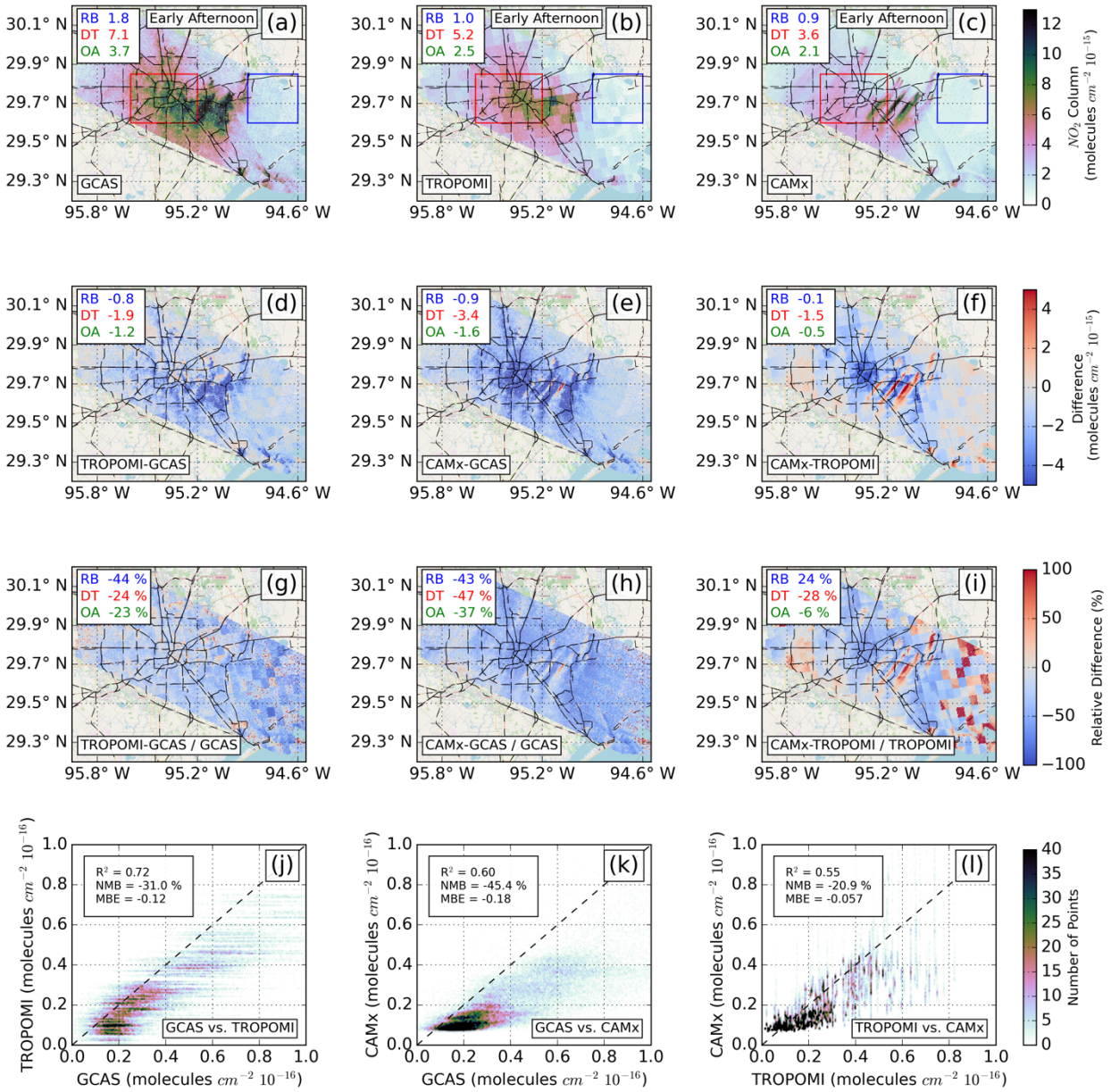

Figure S5: Spatial comparison of GCAS, TROPOMI, and CAMx on September 9, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

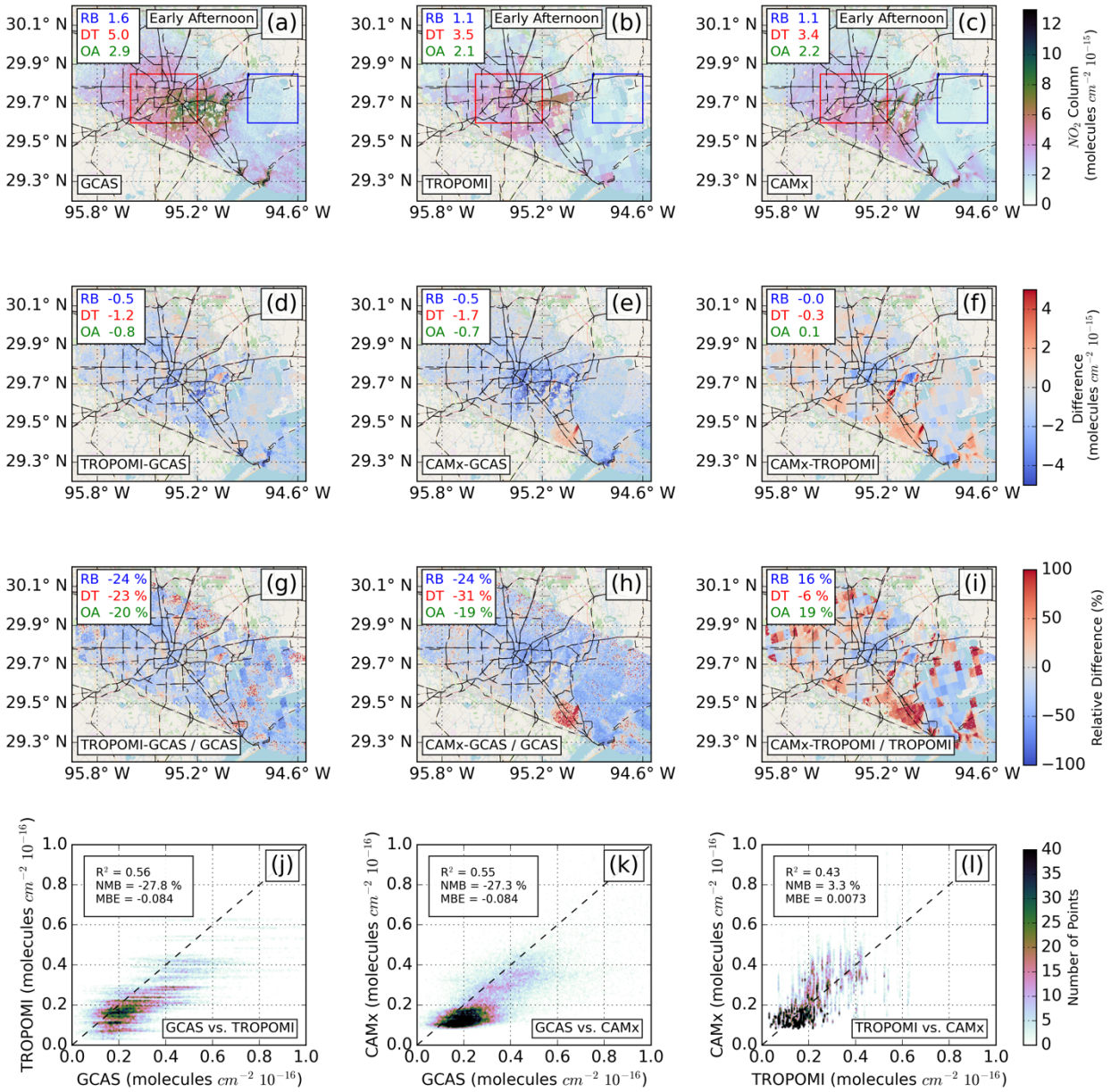

Figure S6: Spatial comparison of GCAS, TROPOMI, and CAMx on September 10, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

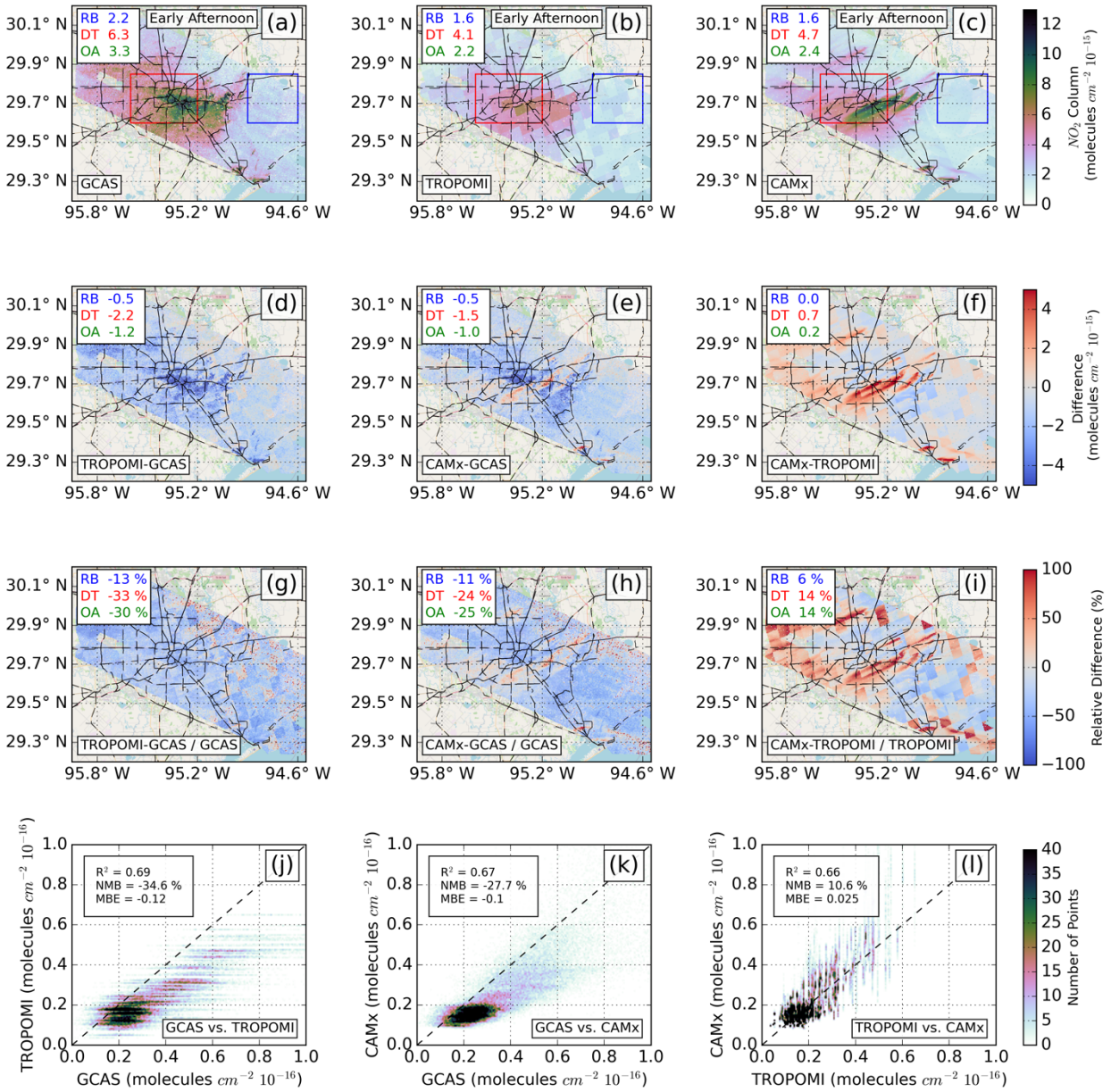

Figure S7: Spatial comparison of GCAS, TROPOMI, and CAMx on September 11, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

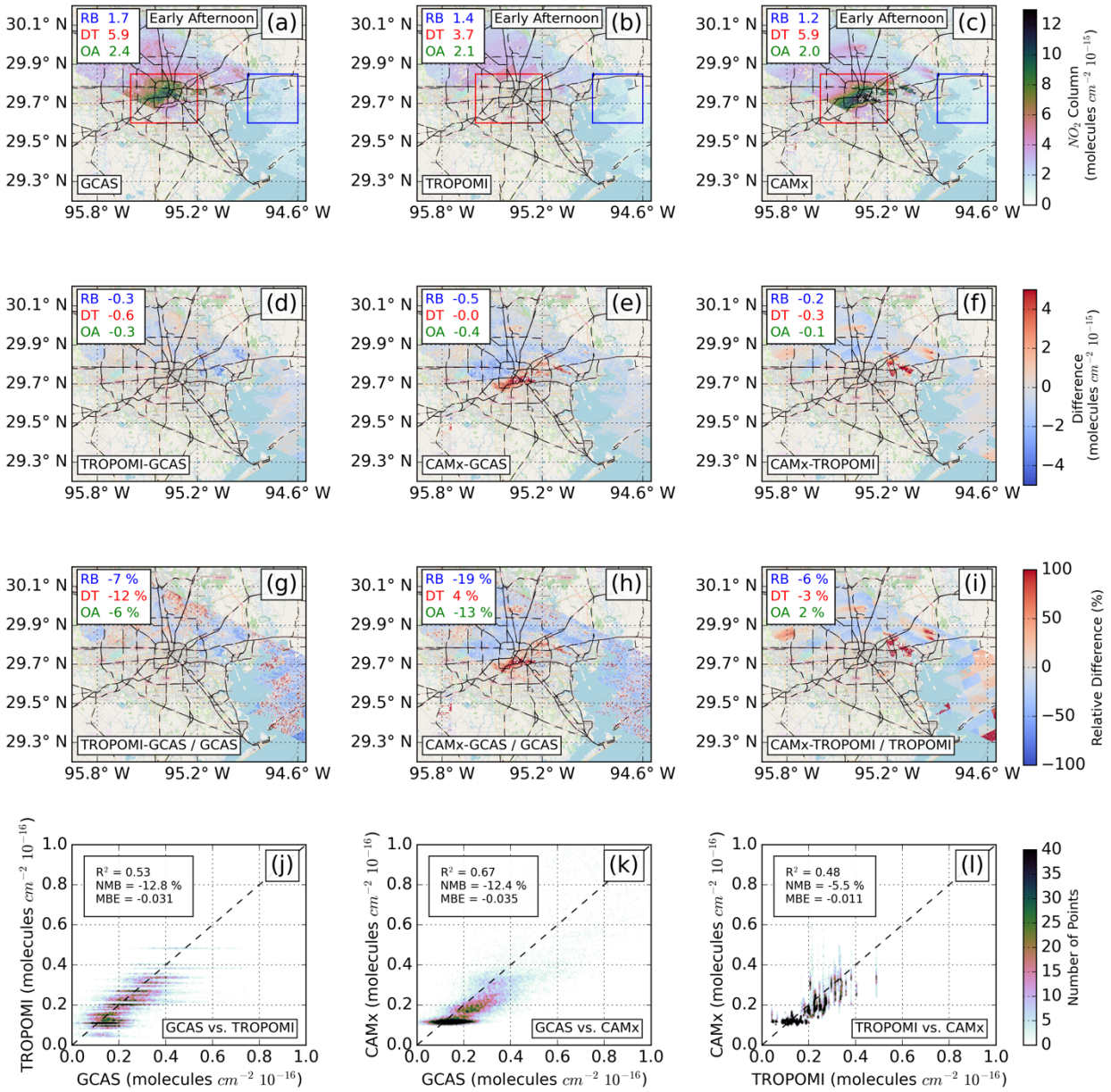

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Figure S8: Spatial comparison of GCAS, TROPOMI, and CAMx on September 23, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

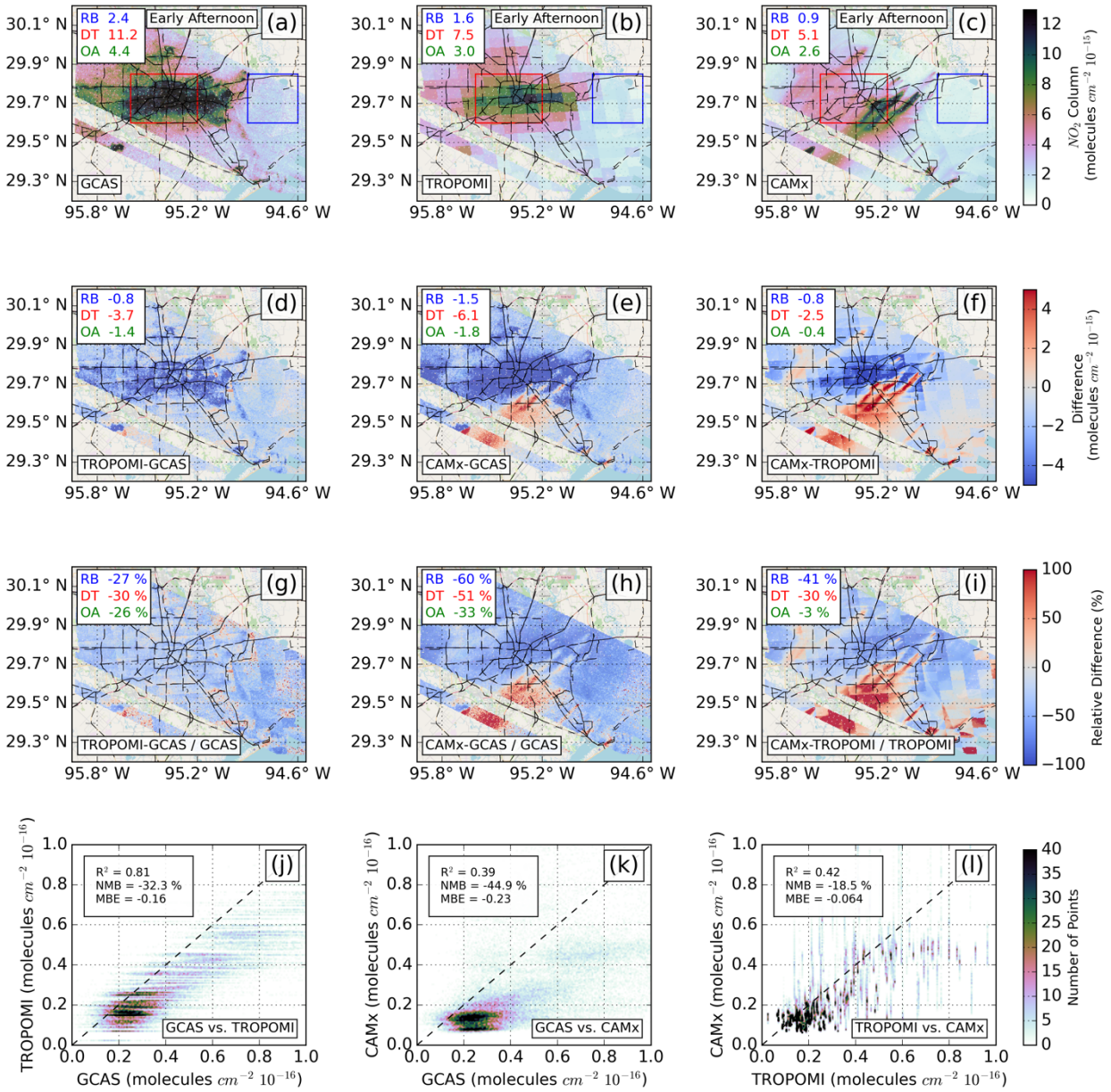

Figure S9: Spatial comparison of GCAS, TROPOMI, and CAMx on September 24, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

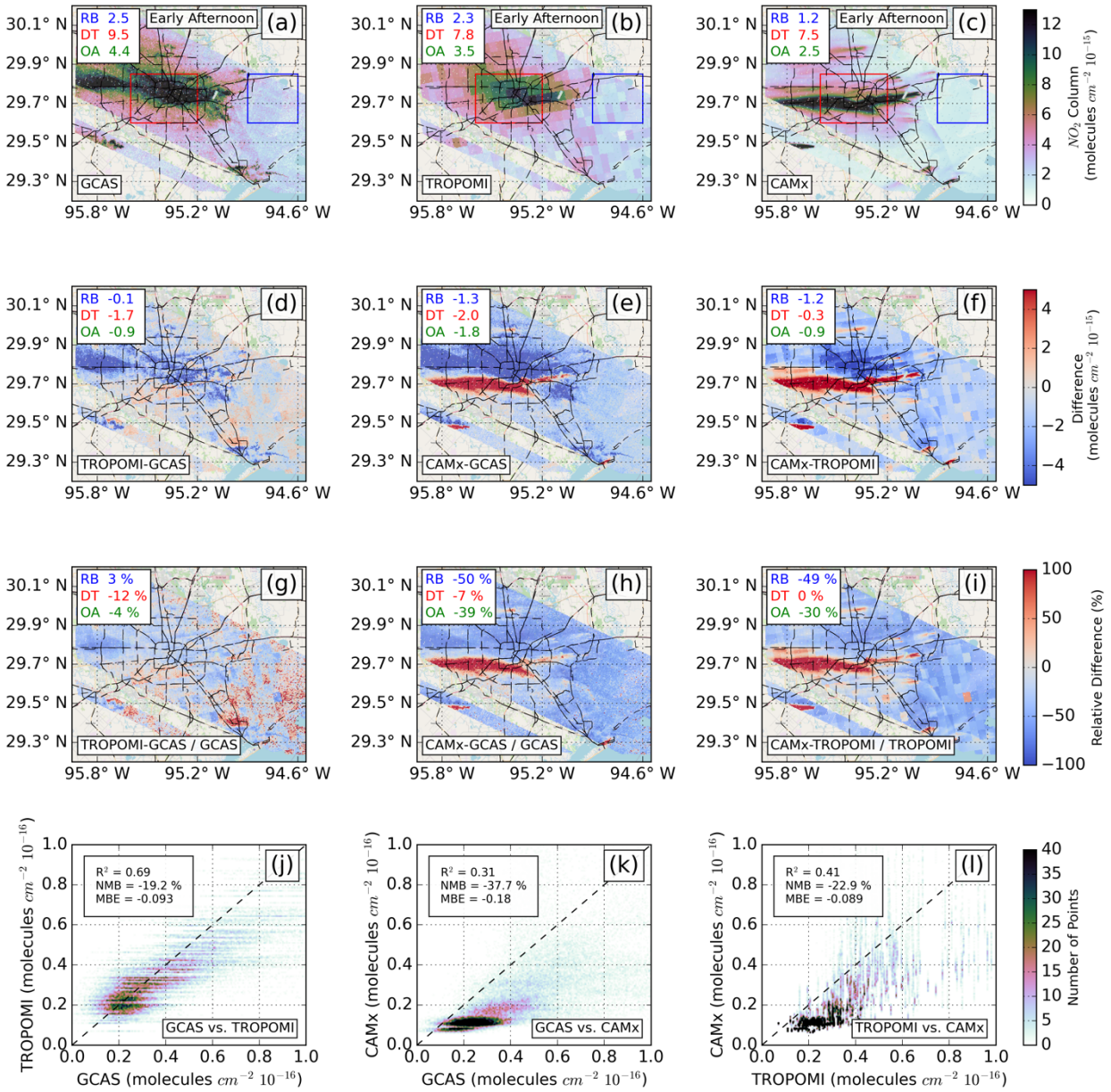

Figure S10: Spatial comparison of GCAS, TROPOMI, and CAMx on September 25, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

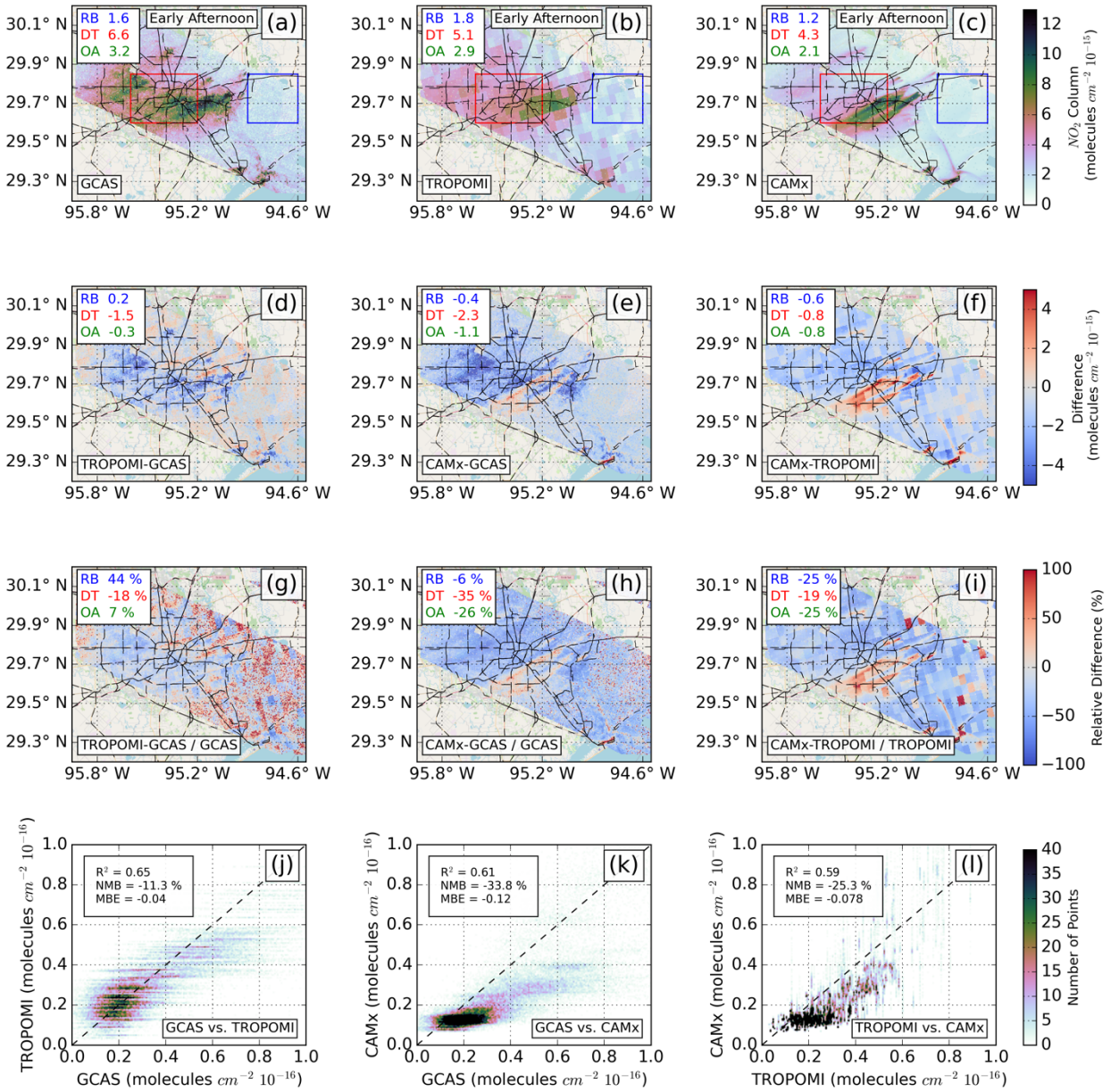

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Figure S11: Spatial comparison of GCAS, TROPOMI, and CAMx on September 26, 2021. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

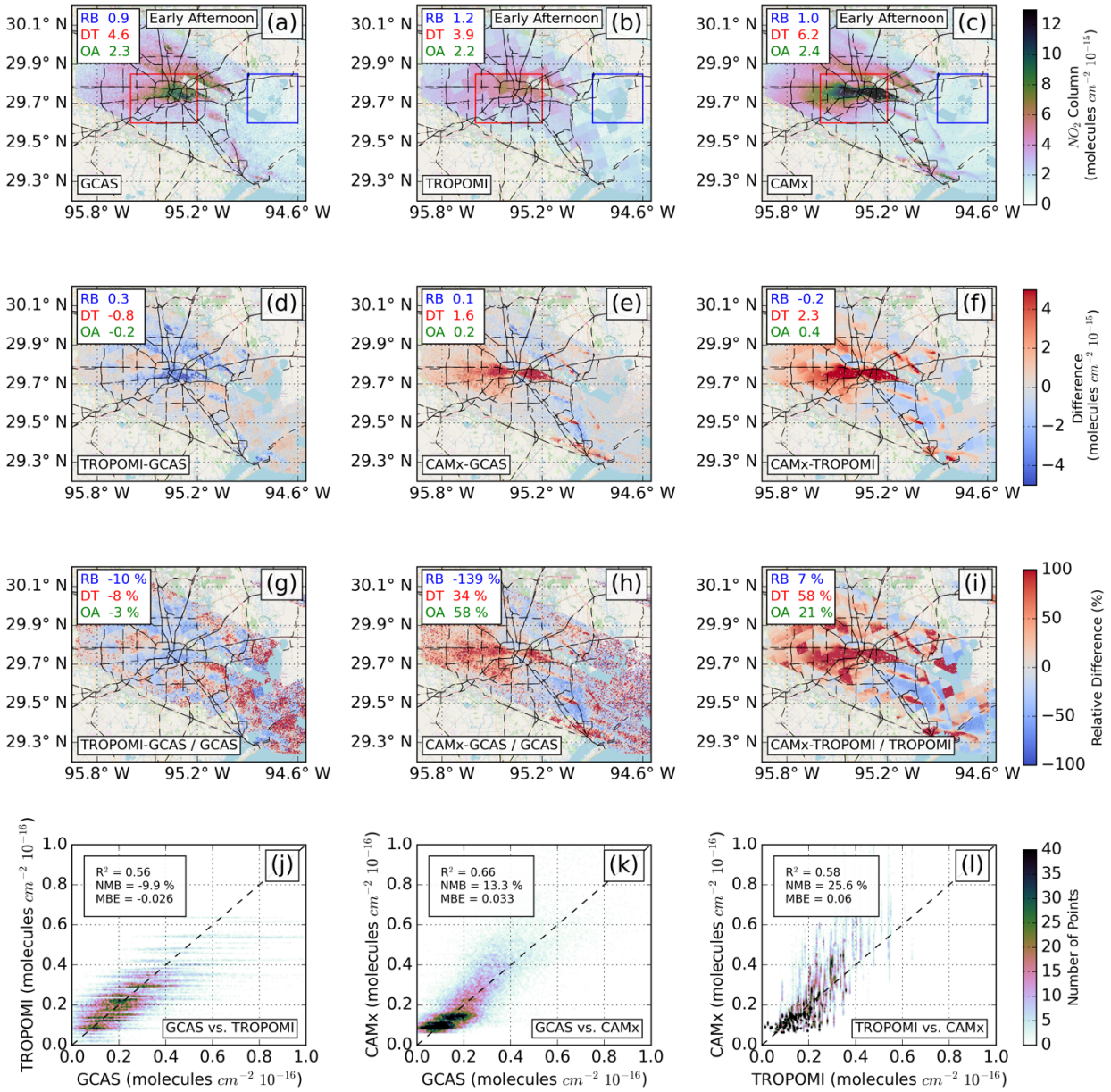

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Figure S12: Map of notable features in and around Houston. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

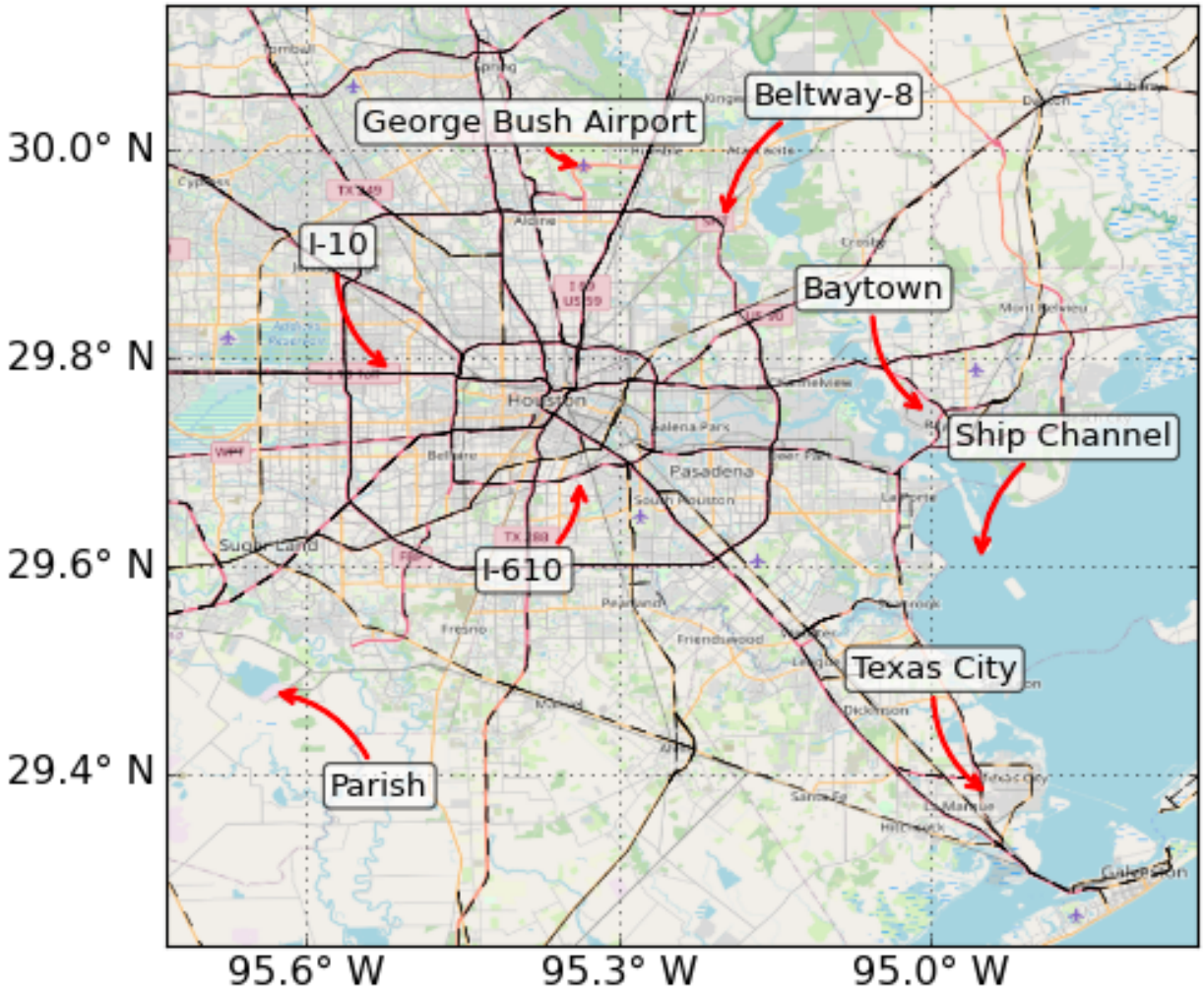

Figure S13: Spatial comparison of GCAS, TROPOMI, and CAMx at the 0.25° × 0.25° resolution. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

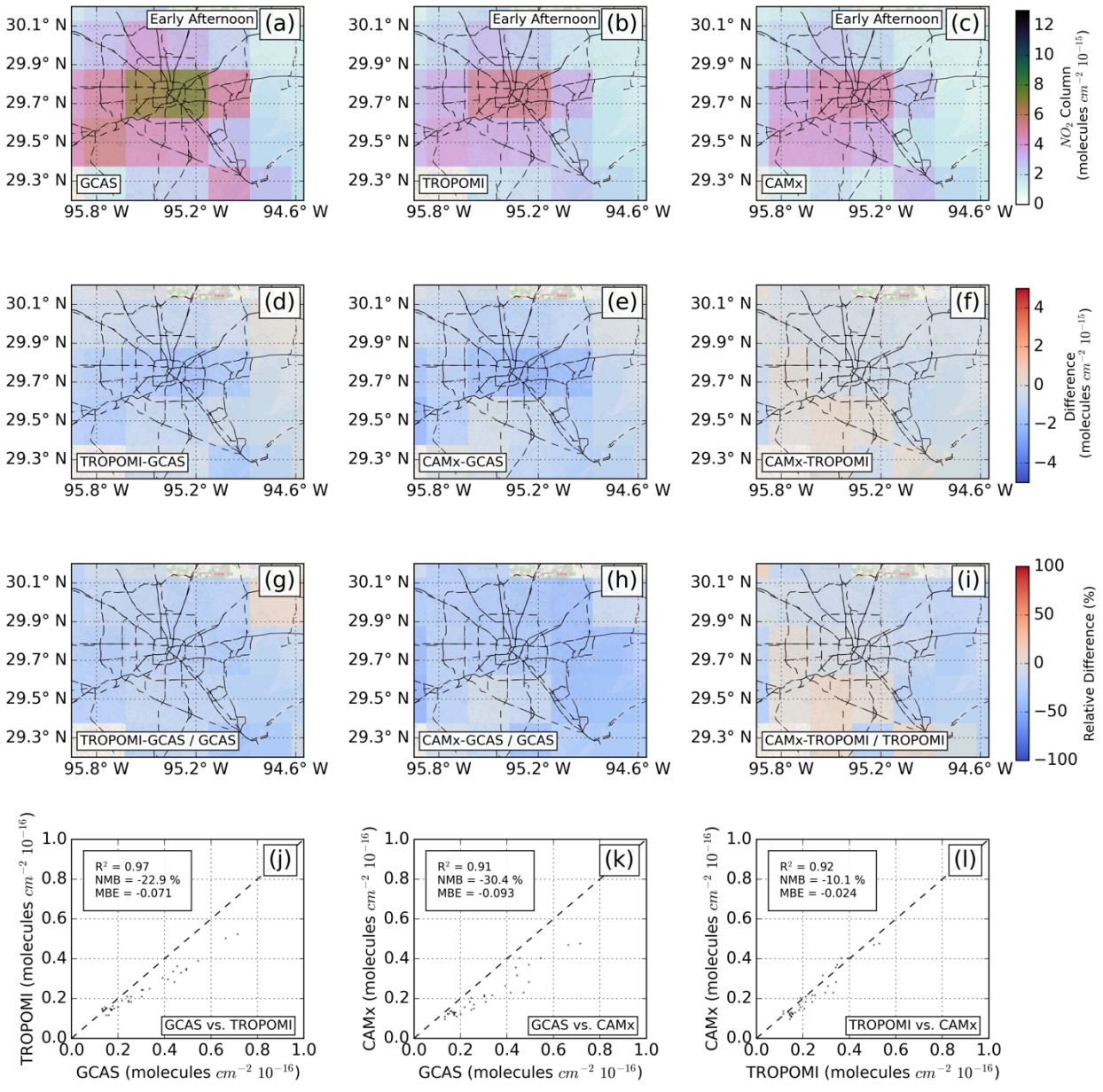

Figure S14: Spatial comparison of GCAS, TROPOMI, and CAMx at the 0.1° × 0.1° resolution. © OpenStreetMap contributors *2023*. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

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