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Supporting Information for

Validation of IASI satellite ammonia observations at the pixel scale using in-situ vertical profiles

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Introduction

This SI provides more details on the comparison between IASI and in-situ columns in Colorado and California. Orthogonal regression was used for all the analyses as mentioned in the main text.

IASI	In-situ	IASI (cont'd)	In-situ (cont'd)
-1.90e15	8.87e15	2.32e15	3.11e15
1.04e15	1.56e16	3.25e15	2.44e15
1.51e16	5.04e15	1.74e16	5.62e15
7.57e15	2.33e16	1.68e16	1.49e16
6.52e15	4.44e15	3.21e16	2.26e16
1.40e16	1.00e16	3.61e15	1.29e16
5.51e15	6.52e15	2.57e15	2.43e15
8.36e15	8.23e15	2.43e15	3.05e15
7.49e15	5.74e15	8.16e15	9.29e15
1.70e16	7.70e15	6.45e15	1.86e15
1.02e16	1.11e16	1.81e16	4.79e15
4.80e15	1.09e16	6.12e15	6.23e15
9.11e15	5.70e15	5.91e15	2.16e15
9.46e15	2.09e16	3.16e15	1.62e15
1.68e16	4.04e15	4.37e15	6.86e15
1.05e16	1.49e16	3.68e15	2.34e14
2.45e16	4.10e16	1.05e16	3.17e15
7.23e15	5.57e14	2.05e15	1.07e15
9.10e15	2.25e16	7.44e15	1.82e15
1.41e16	2.41e16	4.98e15	4.41e15
4.05e15	3.27e15	2.99e15	8.26e14
6.67e15	9.77e15	3.42e15	2.47e15
1.51e16	2.04e16	8.63e14	1.98e15
5.03e15	2.43e15	1.62e16	4.67e15
2.84e16	3.23e16	-5.00e14	3.02e15
7.00e15	2.40e15	9.98e15	5.38e15
3.75e15	1.04e16	2.60e15	2.38e15
8.54e15	3.66e15	1.59e16	1.02e16
2.50e16	1.33e16	2.35e15	1.09e16
3.02e15	5.97e15	9.32e15	4.28e15

Table S1. Near real-time IASI product and corresponding in-situ columns in Colorado based on the ±15 km and ±60 min window and MLH assumption (N = 60). Unit: molecules cm^{-2}.

	20 min			60 min			180 min		
Temporal window									
Spatial window	Within pixel	15 km	45 km	Within pixel	15 km	45 km	Within pixel	15 km	45 km
Slope	N/A	11 ±31	2.3 ±0.43	1.7 ±0.92	4.8 ±4.0	4.1 ±0.81	4.6 ±8.2	4.1 ±4.2	1.6 ±0.21
Intercept	N/A	-1.6e17 ±5.8e17	-8.6e15 ±7.4e15	8.1e15 ±1.4e16	-6.6e16 ±7.8e16	-2.7e16 ±1.0e16	-6.0e16 ±1.6e17	-4.8e16 ±7.3e16	-8.5e15 ±4.3e15
Correlation coefficient	N/A	0.15	0.70	0.67	0.37	0.56	0.27	0.29	0.65
Number of datapoints	1	5	29	4	9	57	4	11	76
IASI mean	5.4e16	3.3e16 ±2.0e16	2.4e16 ±2.3e16	3.0e16 ±1.7e16	2.6e16 ±1.7e16	2.1e16 ±2.4e16	3.0e16 ±1.7e16	2.3e16 ±1.7e16	1.9e16 ±2.3e16
In-situ mean	1.8e16	1.9e16 ±9.5e15	1.4e16 ±1.3e16	1.3e16 ±1.2e16	1.9e16 ±8.0e15	1.2e16 ±9.6e15	1.9e16 ±9.8e15	1.7e16 ±9.9e15	1.7e16 ±1.7e16
% difference	192	76	68	128	36	78	54	34	8.7

Table S2. Orthogonal regression statistics between the reanalysis IASI product and the in-situ MLH assumption in California for all the spatiotemporal windows tested, including overlapping points.

Temporal window	20 min			60 min			180 min		
Spatial window	Within pixel	15 km	45 km	Within pixel	15 km	45 km	Within pixel	15 km	45 km
Slope	1.2 ±0.18	1.0 ±0.19	0.11 ±0.04	3.0 ±1.2	1.0 ±0.19	1.5 ±0.23	3.2 ±0.66	3.5 ±0.77	0.66 ±0.11
Intercept	-2.2e13 ±2.5e15	3.8e13 ±2.9e15	8.9e15 ±8.0e14	-1.0e16 ±8.7e15	1.3e15 ±1.9e15	-1.4e15 ±1.7e15	-7.6e15 ±4.5e15	-1.1e16 ±5.3e15	4.1e15 ±7.8e14
Correlation coefficient	0.88	0.74	0.22	0.45	0.57	0.39	0.65	0.44	0.35
Number of datapoints	12	23	151	26	63	240	33	84	248
IASI mean	1.2e16 ±1.2e16	1.2e16 ±1.1e16	1.0e16 ±8.6e15	1.1e16 ±9.2e15	1.0e16 ±8.4e15	8.5e15 ±7.9e15	1.2e16 ±1.0e16	1.1e16 ±1.0e16	7.9e15 ±6.9e15
In-situ mean	1.1e16 ±1.0e16	1.2e16 ±1.1e16	1.1e16 ±2.1e16	7.1e15 ±5.2e15	8.8e15 ±8.2e15	6.8e15 ±6.8e15	6.1e15 ±4.5e15	6.4e15 ±5.1e15	5.7e15 ±8.0e15
% difference	15	-0.14	-7.4	56	19	26	96	74	39

Table S3. Orthogonal regression statistics between the reanalysis IASI product and the in-situ MLH assumption in Colorado for all the spatiotemporal windows tested, including overlapping points.

Temporal window	20 min			60 min			180 min		
Spatial window	Within pixel	15 km	45 km	Within pixel	15 km	45 km	Within pixel	15 km	45 km
Slope	1.2 ±0.18	1.0 ±0.23	0.16 ±0.05	3.5 ±1.4	1.1 ±0.22	1.5 ±0.25	3.2 ±0.63	3.6 ±0.78	1.1 ±0.22
Intercept	2.9e14 ±2.6e15	5.1e14± 3.5e15	9.3e15 ±8.5e14	-1.1e16 ±9.7e15	1.7e15 ±2.2e15	-1.4e15 ±1.8e15	-6.3e15 ±4.0e15	-1.0e16 ±5.1e15	2.3e15 ±1.4e15
Correlation coefficient	0.89	0.68	0.28	0.45	0.54	0.37	0.67	0.46	0.30
Number of datapoints	12	22	151	25	60	243	32	80	258
IASI mean	1.3e16 ±1.2e16	1.3e16 ±1.1e16	1.1e16 ±9.0e15	1.1e16 ±1.0e16	1.1e16 ±8.7e15	9.0e15 ±8.1e15	1.2e16 ±1.0e16	1.2e16 ±1.0e16	8.8e15 ±8.6e15
In-situ mean	1.1e16 ±1.0e16	1.3e16 ±1.1e16	1.0e16 ±1.9e16	6.6e15 ±5.1e15	8.5e15 ±8.2e15	6.7e15 ±6.8e15	5.7e15 ±4.4e15	6.2e15 ±5.0e15	5.9e15 ±8.4e15
% difference	24	4.3	7.5	74	30	33	111	88	51

Table S4. Orthogonal regression statistics between the in-situ derived IASI product and the in-situ MLH assumption in Colorado for all the spatiotemporal windows tested, including overlapping points.