Improved Analysis of VOC, NO_2, SO_2 and HCHO Data from SOF, Mobile DOAS and MW-DOAS during DISCOVER-AQ

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Department of Earth and Atmospheric Sciences
University of Houston

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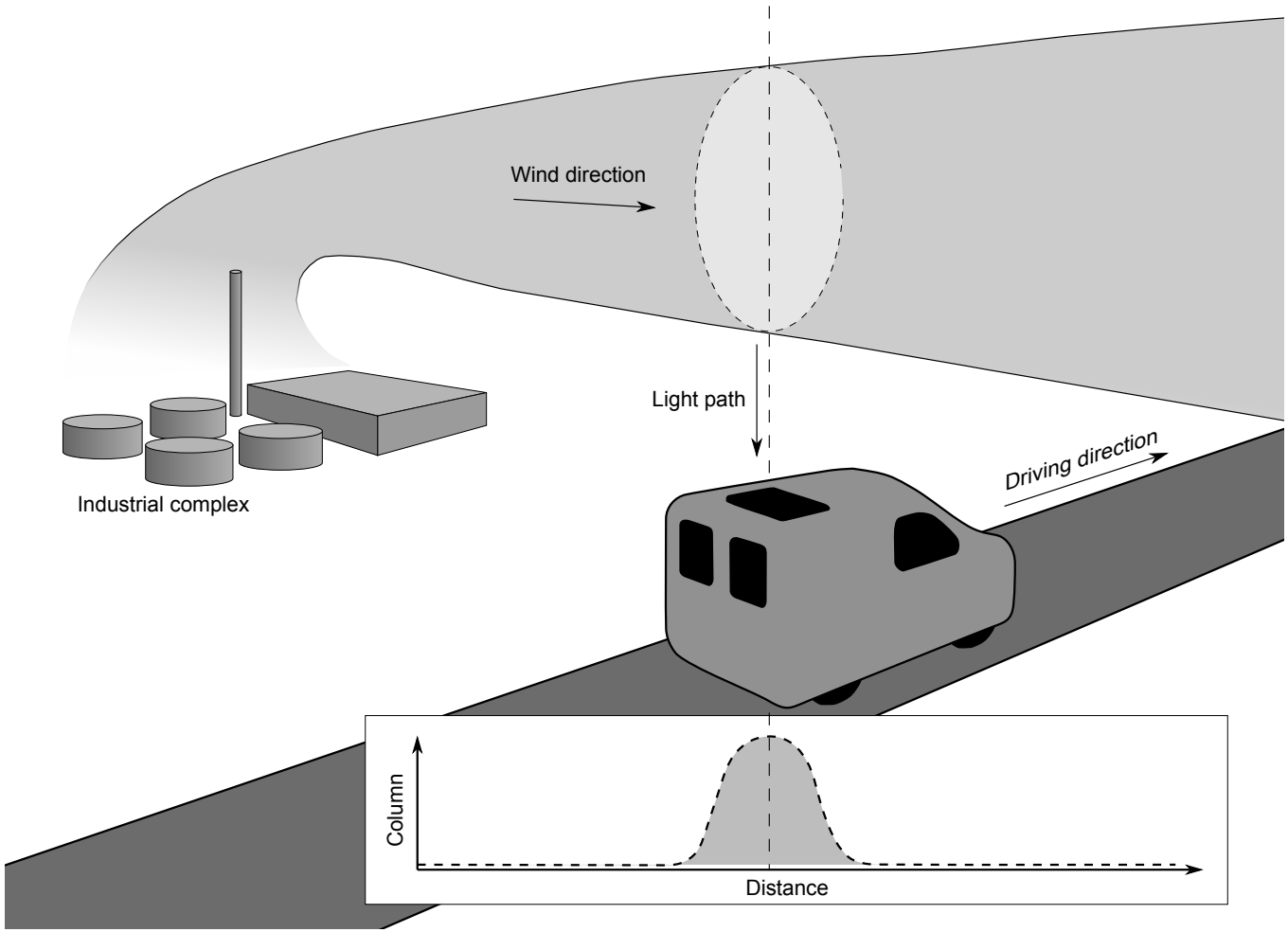
The SOF platform

SOF Mobile lab:

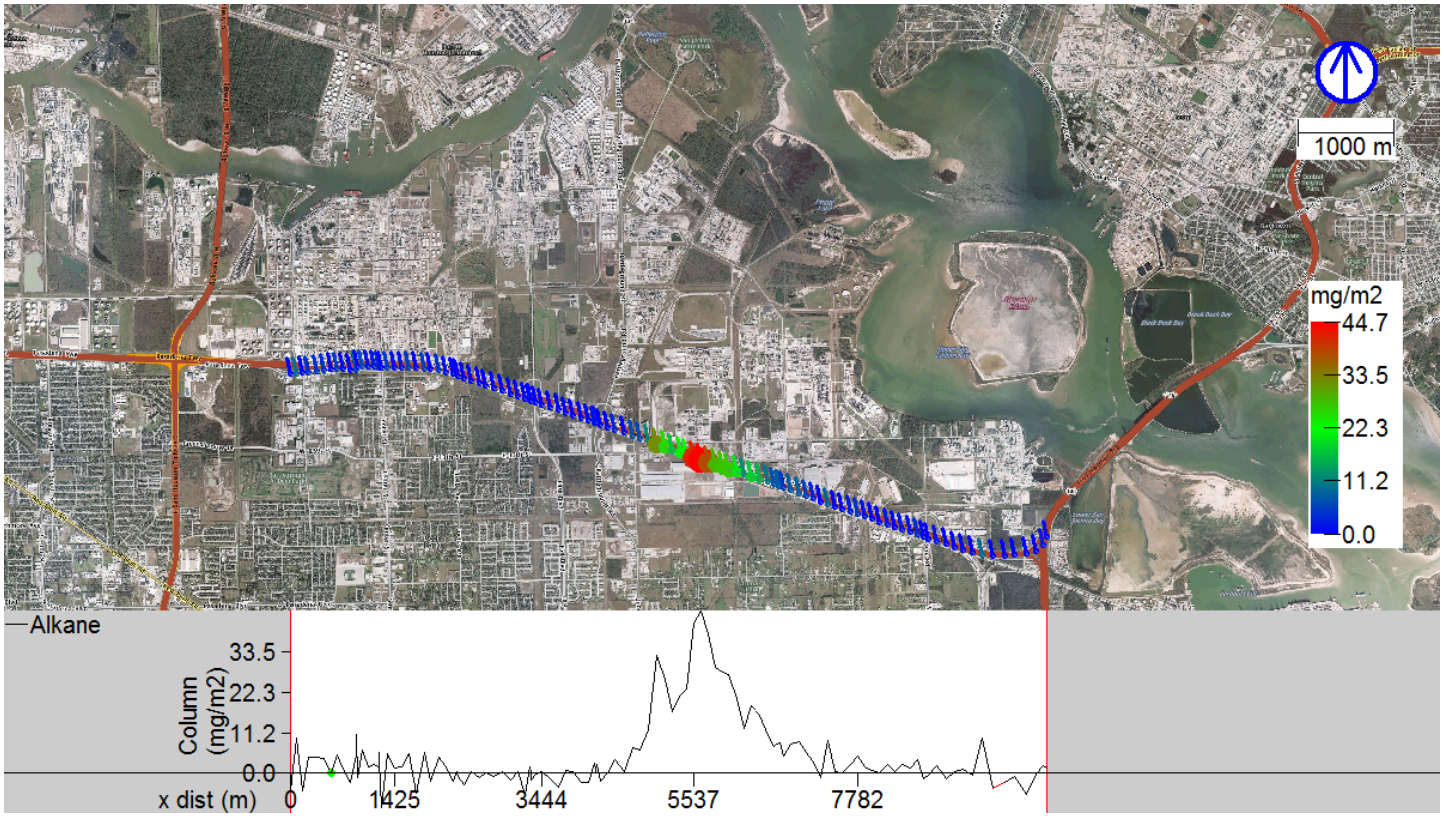
Flux measurements

Principle of measurements:



Propene transect

Example measurement:



Miller Cutoff Rd 25 Sep: ~150 kg/h

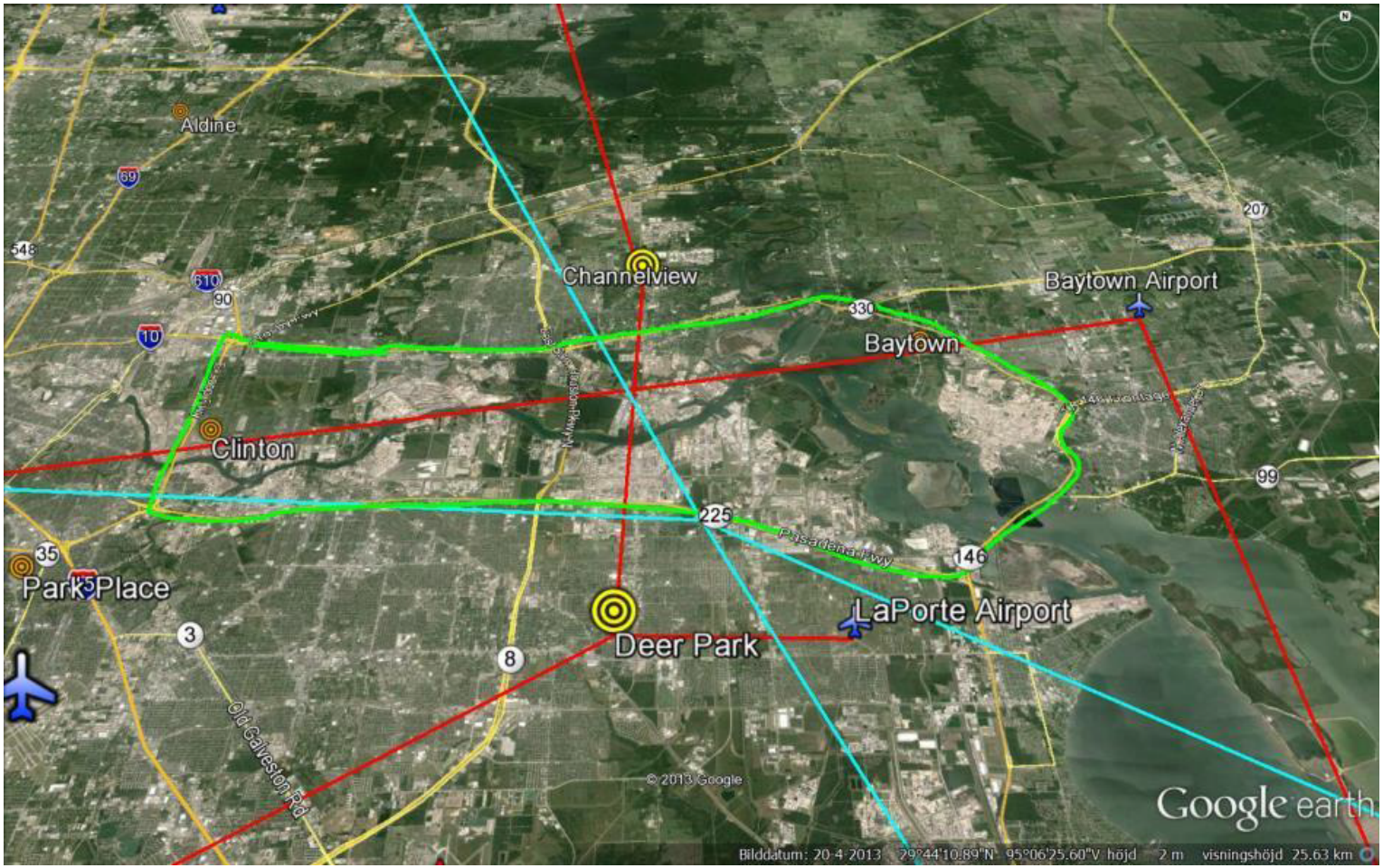
Summary of results

Comparison to inventories and previous campaigns:

Area	Species	2006	2009	2011	2013	EI 2011
HSC	Ethene	878 ± 152	614 ± 284	612 ± 168	474.9 ± 79.3	53
	Propene	1511 ± 529	642 ± 108	563 ± 294*	394 ± 245	63
	Alkanes	12276 ± 3491	10522 ± 2032	11569 ± 2598	13934 ± 4321	894
	SO_2	2277 ±1056	3364 ± 821	2329 ± 466	1955 ± 376	1228
	NO_2	2460 ± 885	-	1830 ± 330	2117 ± 672	1103
Mont Belvieu	Ethene	443 ± 139	444 ± 174	545 ± 284	271 ± 33	47
	Propene	489 ± 231	303 ± 189	58*	220 ± 115	25
	Alkanes	874	1575 ± 704	1319 ± 280	2854 ± 1212**	127
	NO_2	-	168 ± 39	305 ± 29	261 ± 91	155
Texas City	Ethene	83 ± 12	122 ± 41	177 ± 48	-	2
	Propene	ND	54 ± 22	56 ± 9*	-	6
	Alkanes	3010 ± 572	2422 ± 288	2342 ± 805	1340 ± 140	242
	SO_2	-	834 ± 298	1285 ± 428	442 ± 134	109
	NO_2	460 ± 150	283 ± 30	492 ± 71	371 ± 55	352

Measurement routes

Coordinated with airborne DISCOVER-AQ measurements:



Measurement days

- Few good measurement days
- Trade-off between goals
- Less emission data than previous studies

Date	DISCOVER-AQ flight day	Independent SOF day	Weather conditions
Sep 3		X	Moderate
Sep 4	X		Poor
Sep 6	X		Poor
Sep 8		X (afternoon)	Moderate
Sep 9		X	Moderate
Sep 10		X	Poor
Sep 11	X		Moderate
Sep 12	X		Moderate/good
Sep 13	X		Moderate/poor
Sep 14	X		Poor
Sep 15		X	Poor
Sep 16		X	Poor
Sep 18		X	Moderate
Sep 22		X	Moderate
Sep 23		X (afternoon)	Moderate
Sep 24	X		Moderate/good
Sep 25	X		Good
Sep 26	X		Good
Sep 27	X		Poor
Sep 28		X	Poor

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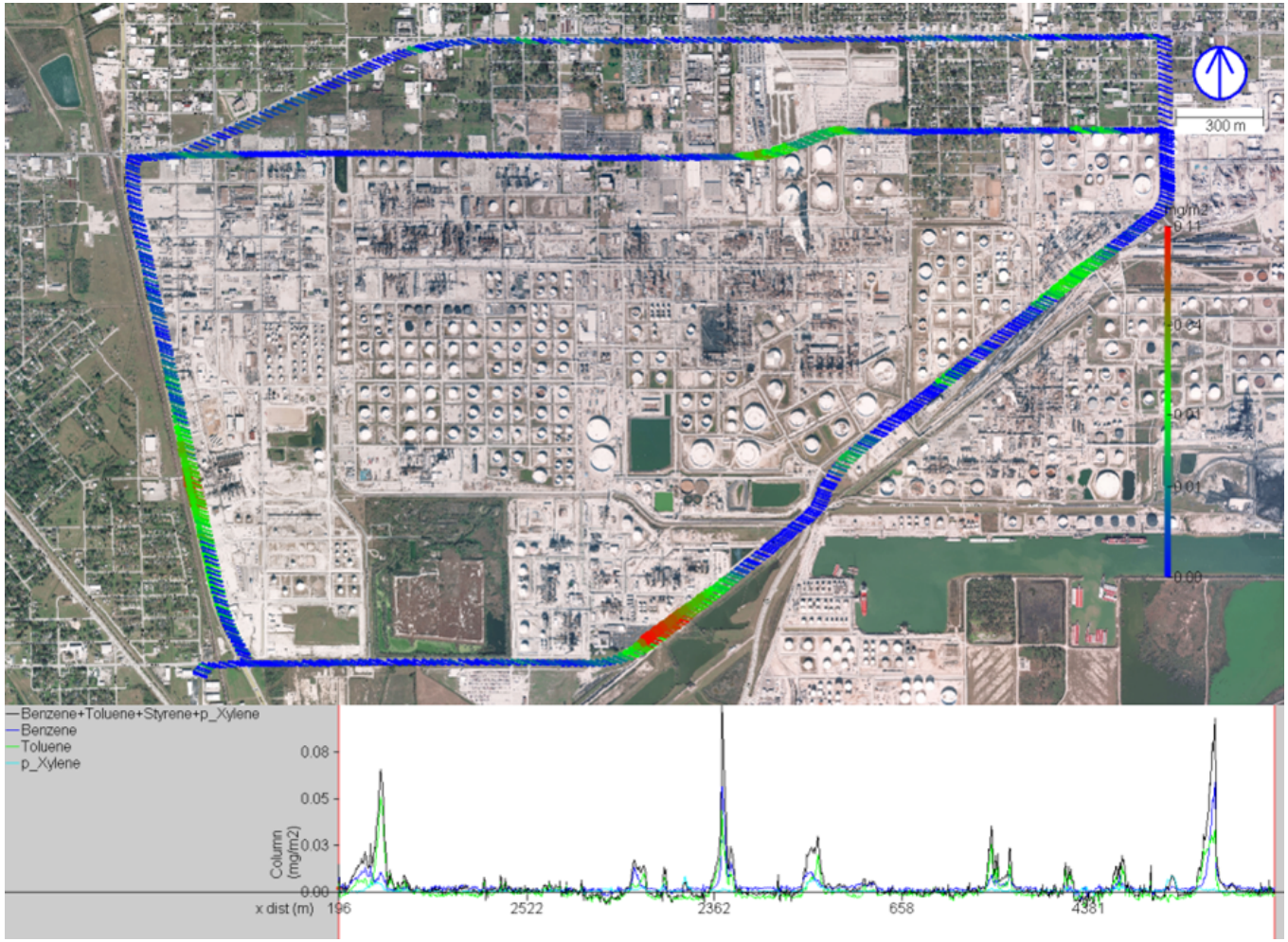
MW-DOAS

Used to quantify aromatic VOC fraction in plumes:



Data analysis project

Project objectives:

- Compare DOAS columns to DISCOVER-AQ data
  - Requires absolute columns . . .
  - . . . and long term stable evaluations
- Investigate cloud effects on measurements
- Improve flux estimates and compare to inventories
- Estimate aromatic emissions from industries

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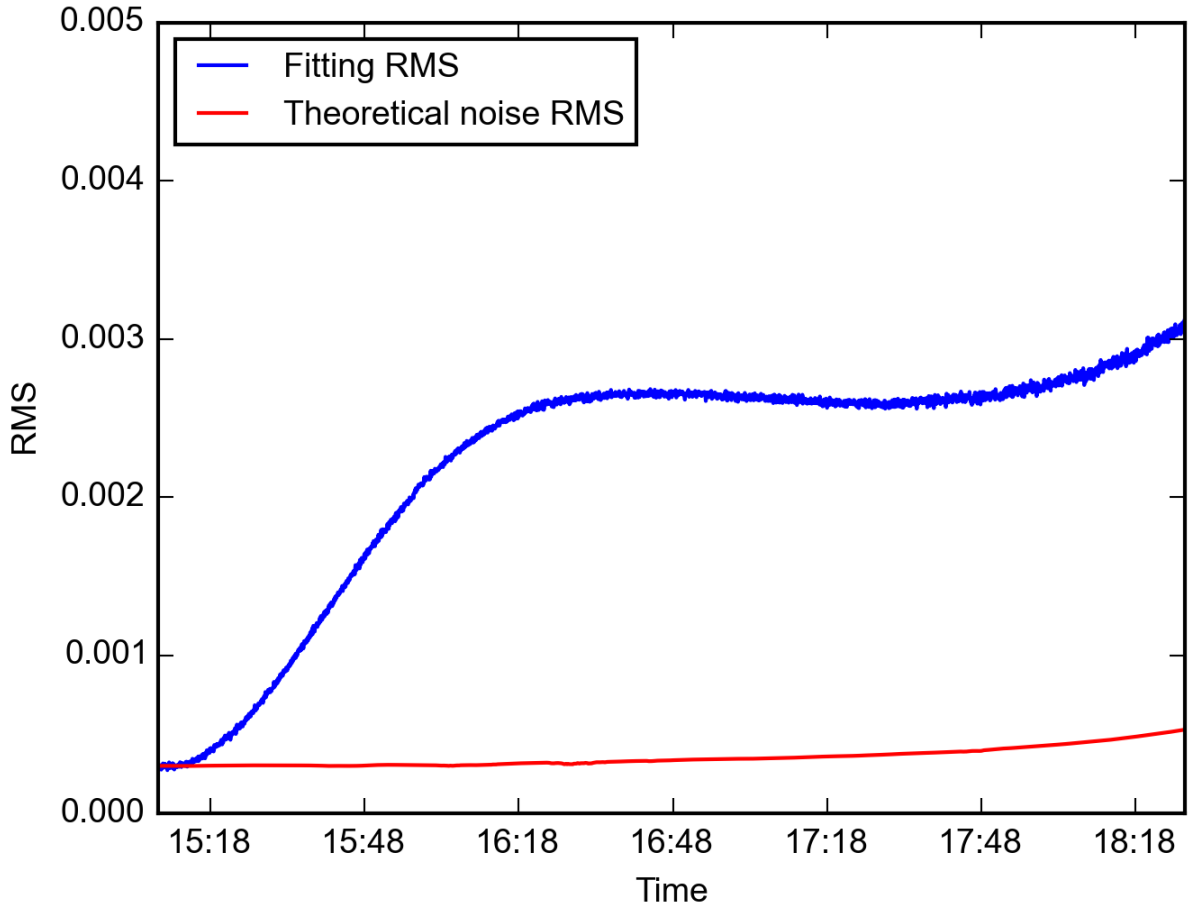
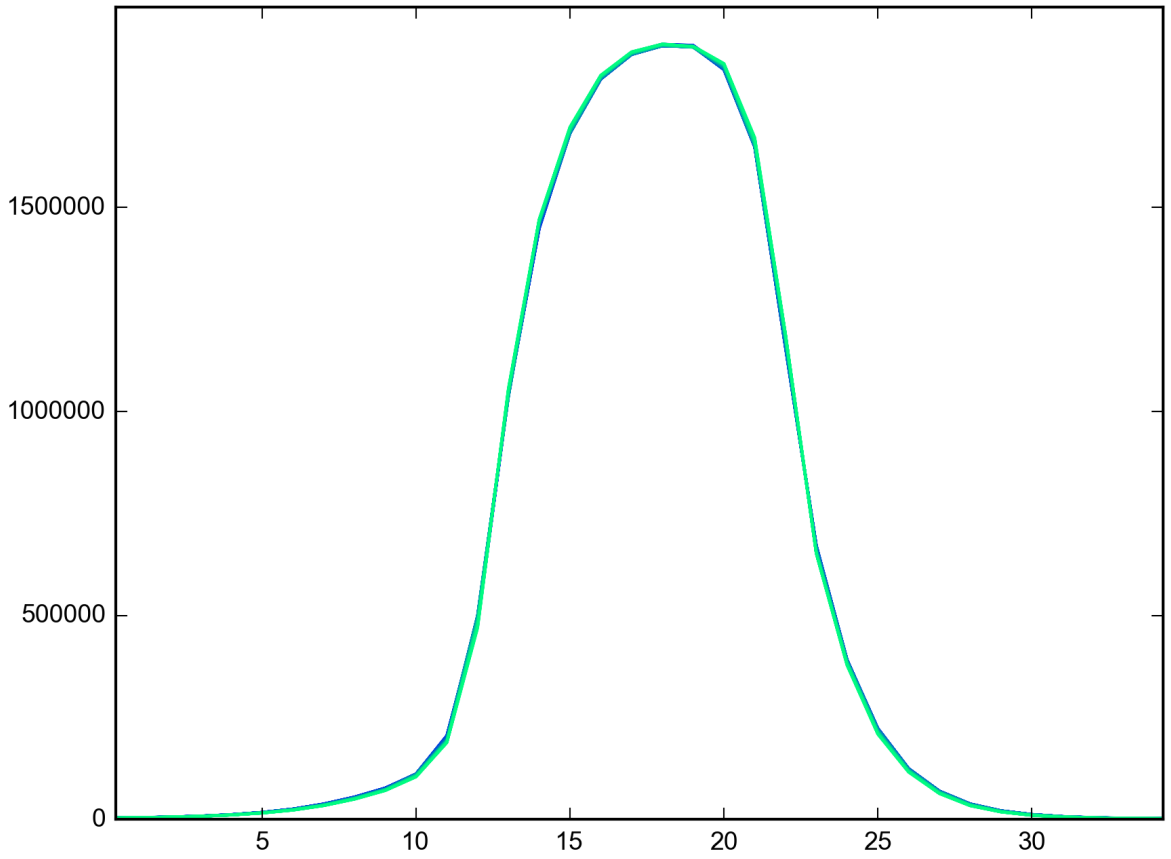
Cloud test measurements

Tests revealed instrumental drift effect. Fitting error (RMS) time series during a test measurement:



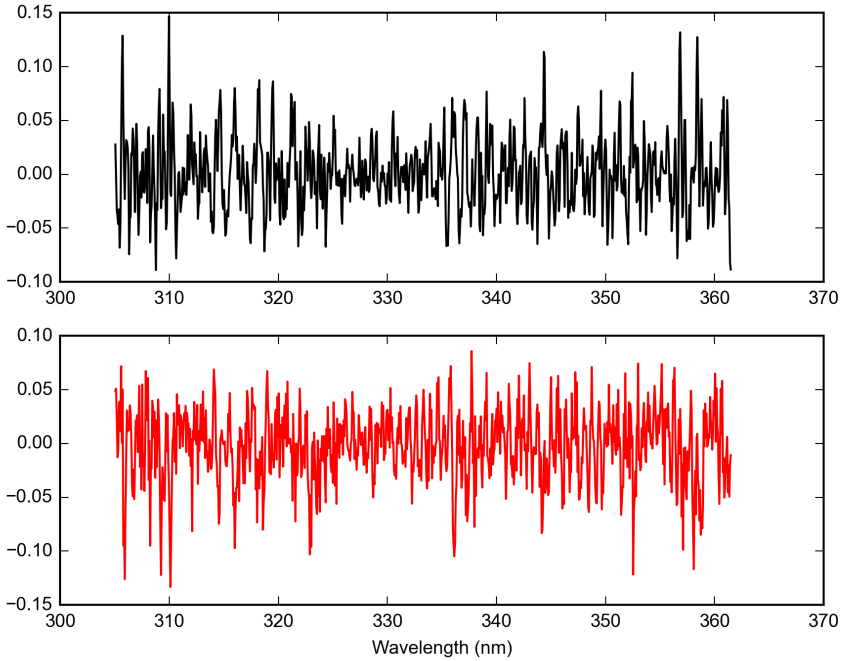
Mercury lamp measurements

Small changes in instrument line shape over time:



Drift correction

- Spectral artifacts due to Fraunhofer lines
- Simulated with synthesized spectra
- Pseudo-absorbers derived by principal component analysis



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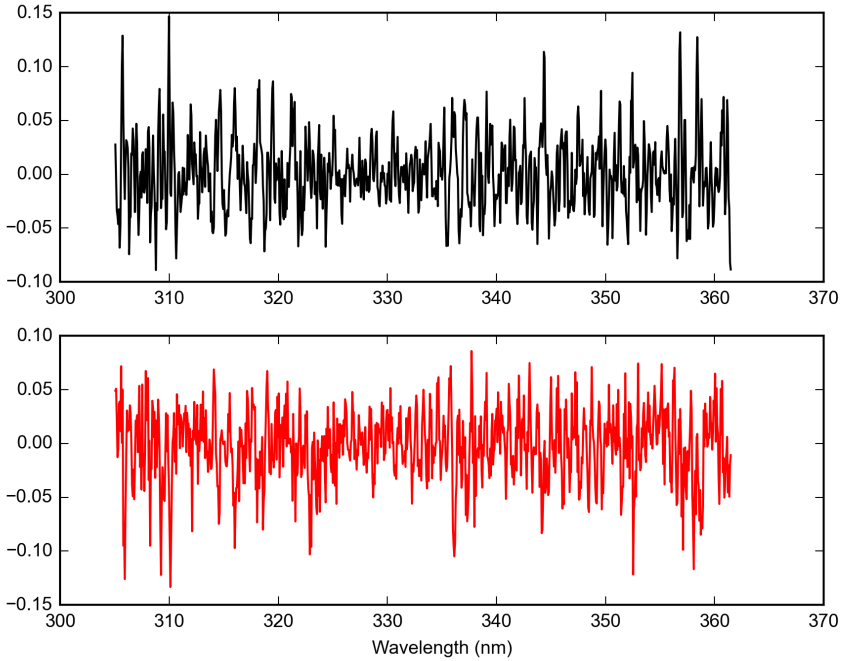

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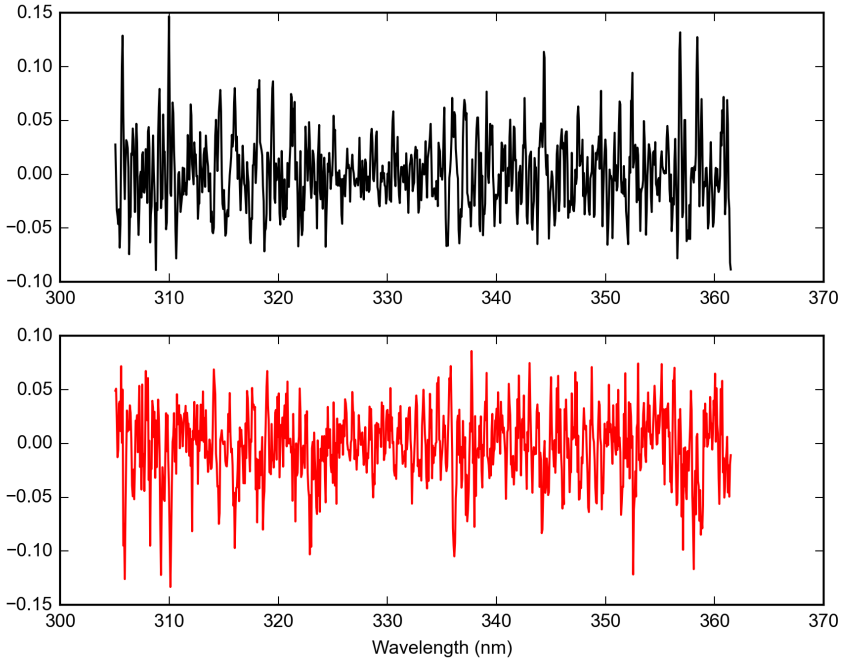
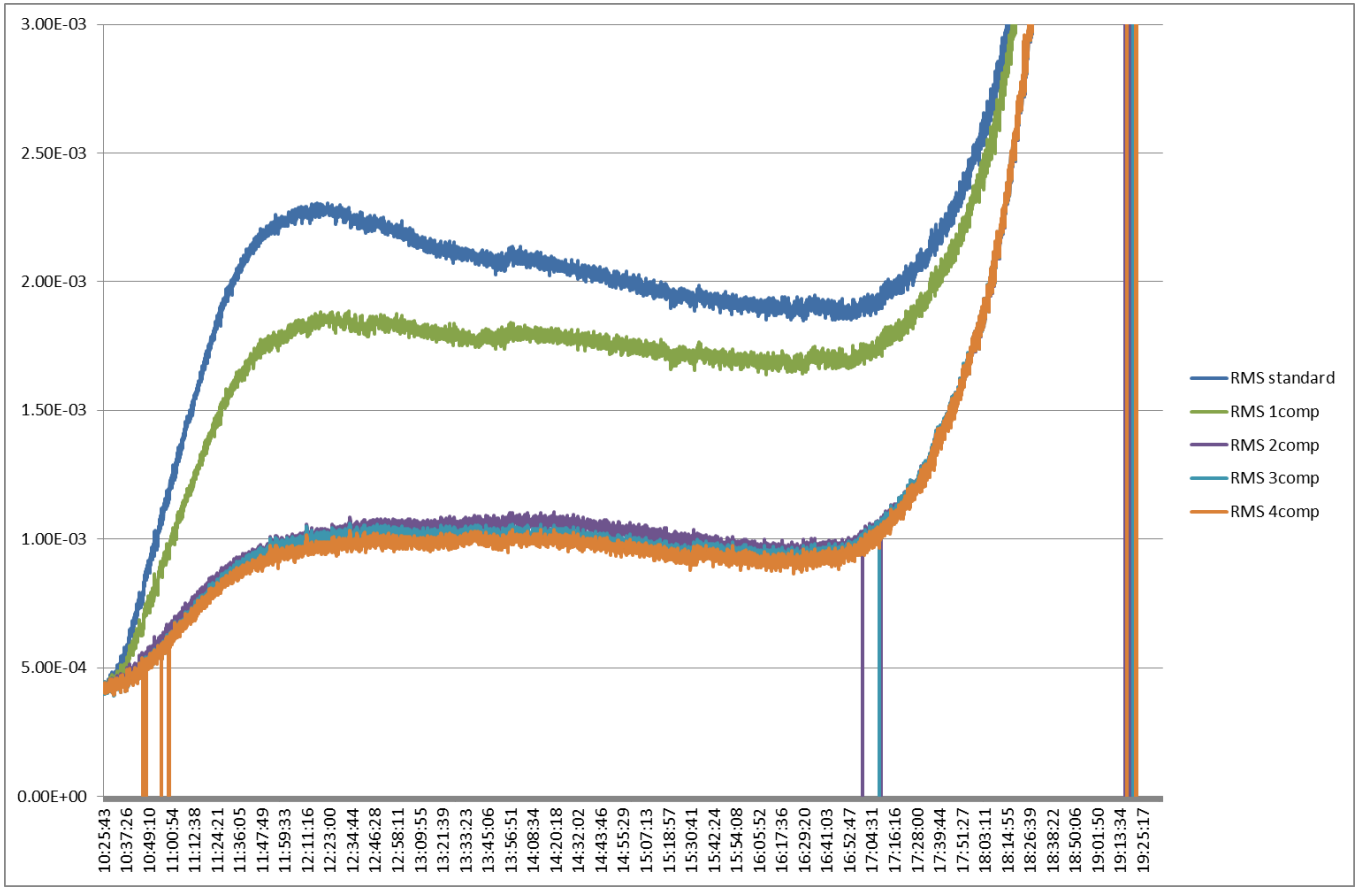


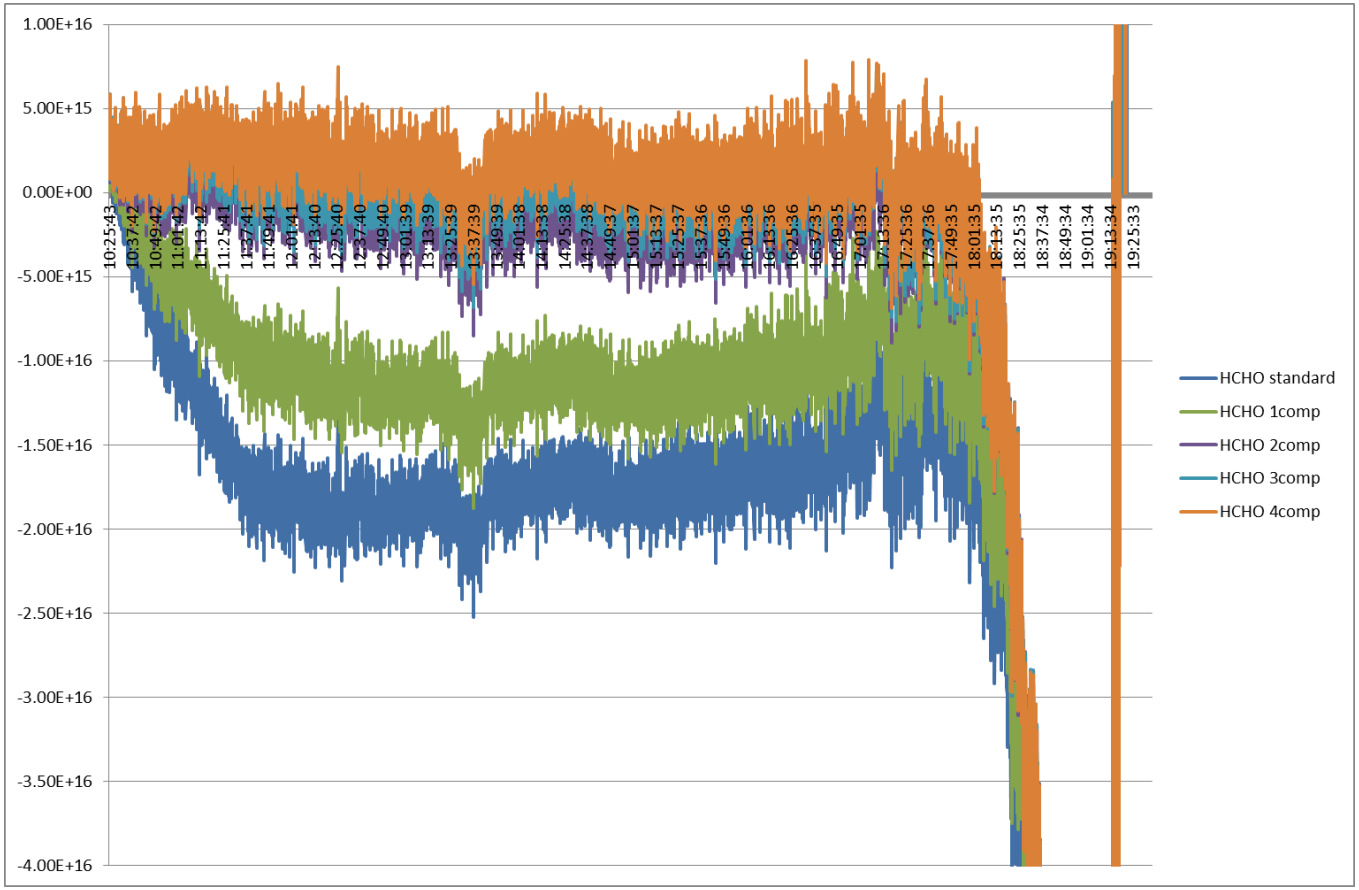
Drift correction

Effect on RMS error:



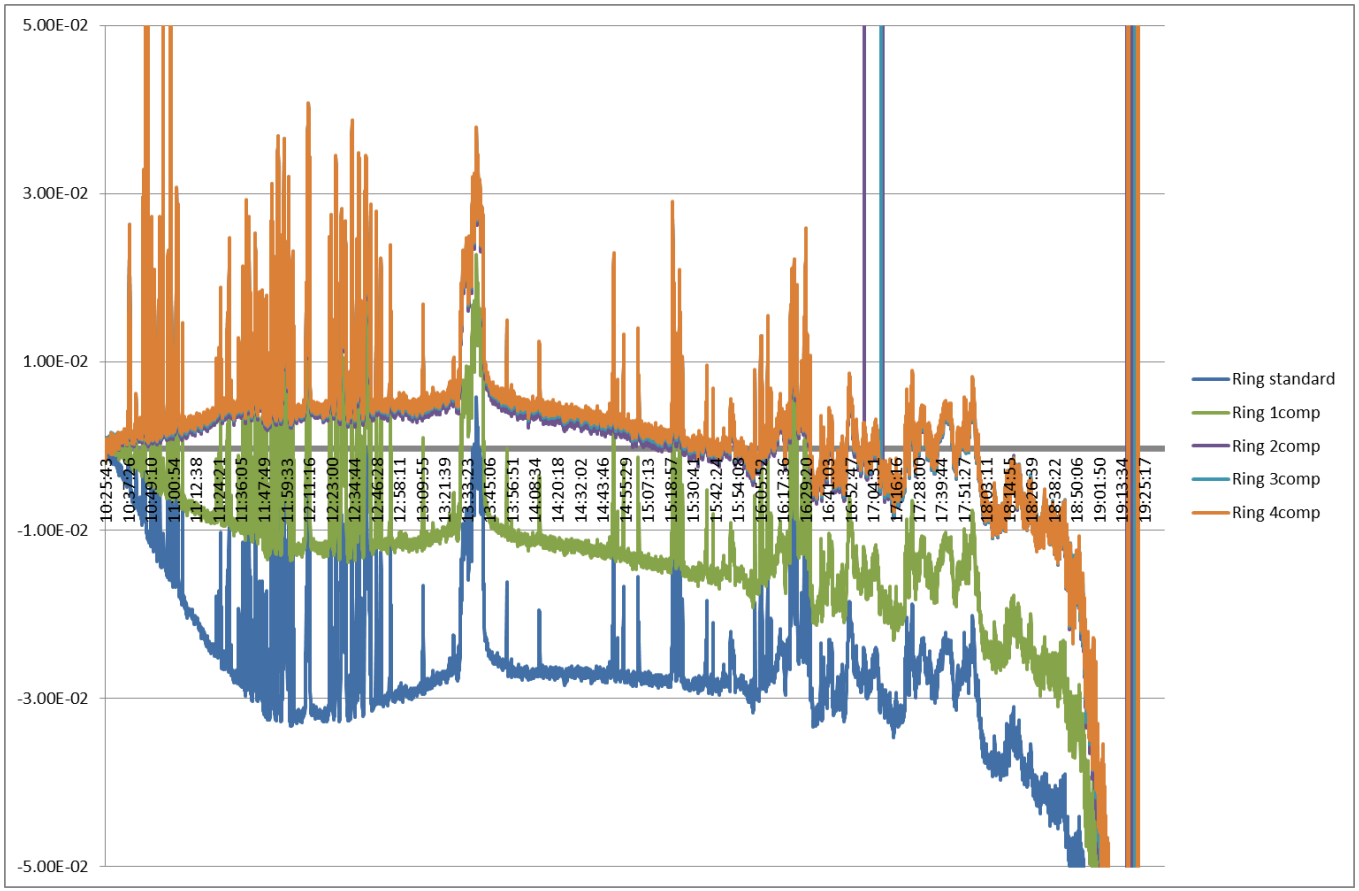
Drift correction

Effect on HCHO columns:



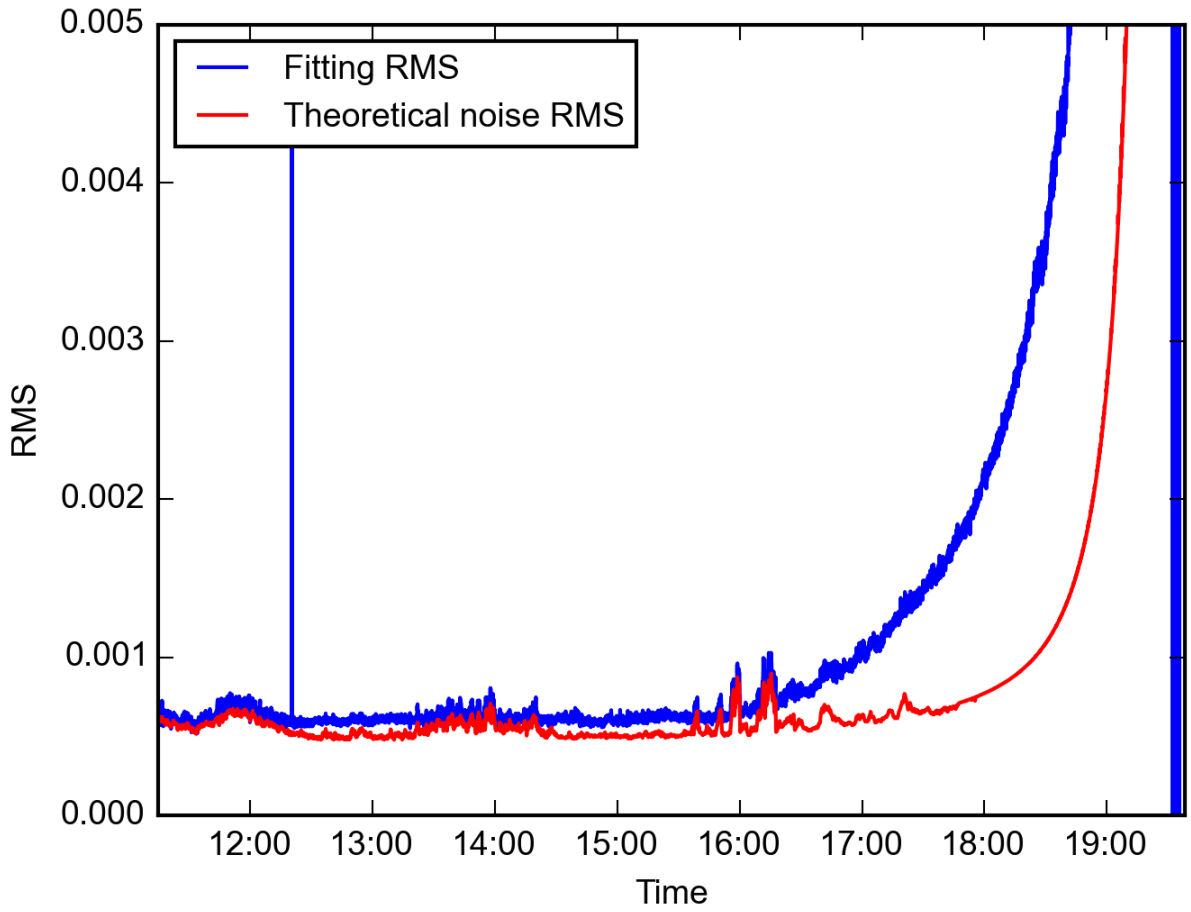
Drift correction

Effect on Ring component:



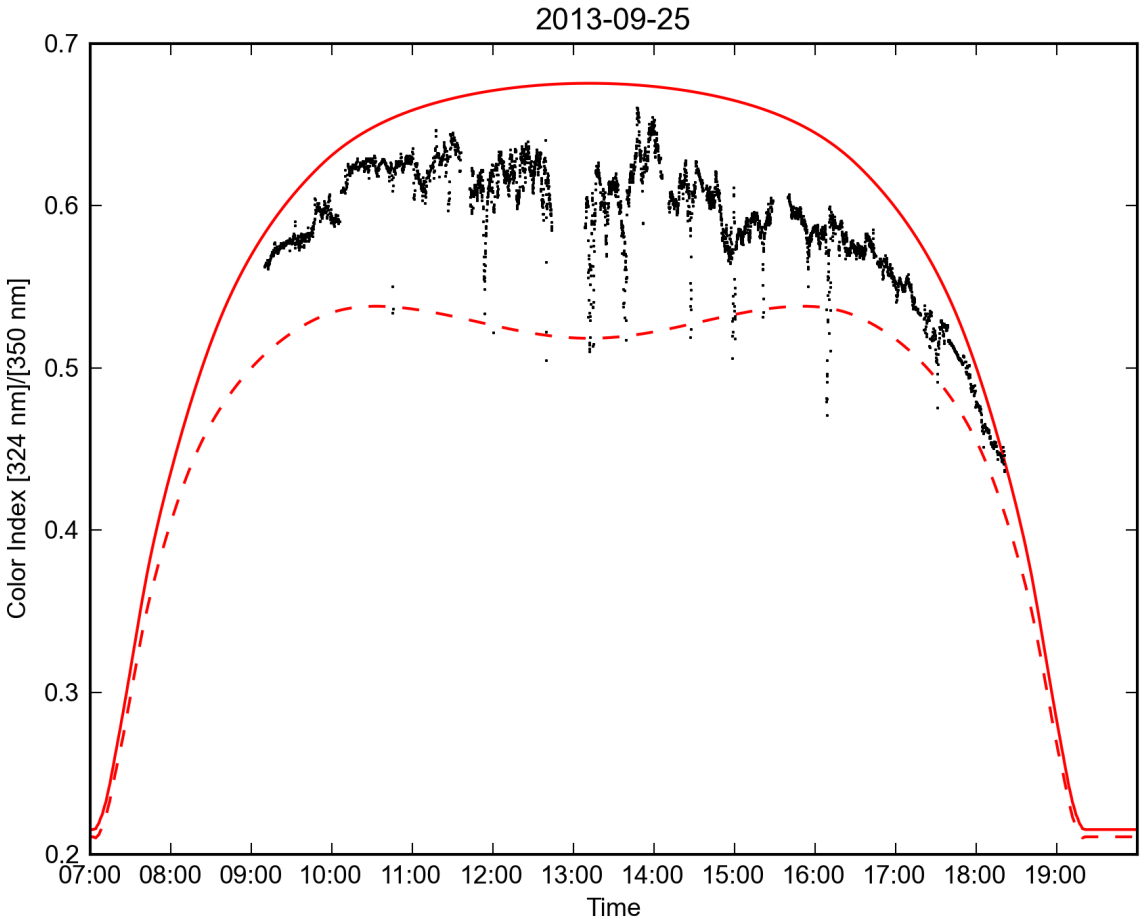
Cloud test measurements

No effect of clouds on spectral fit quality:



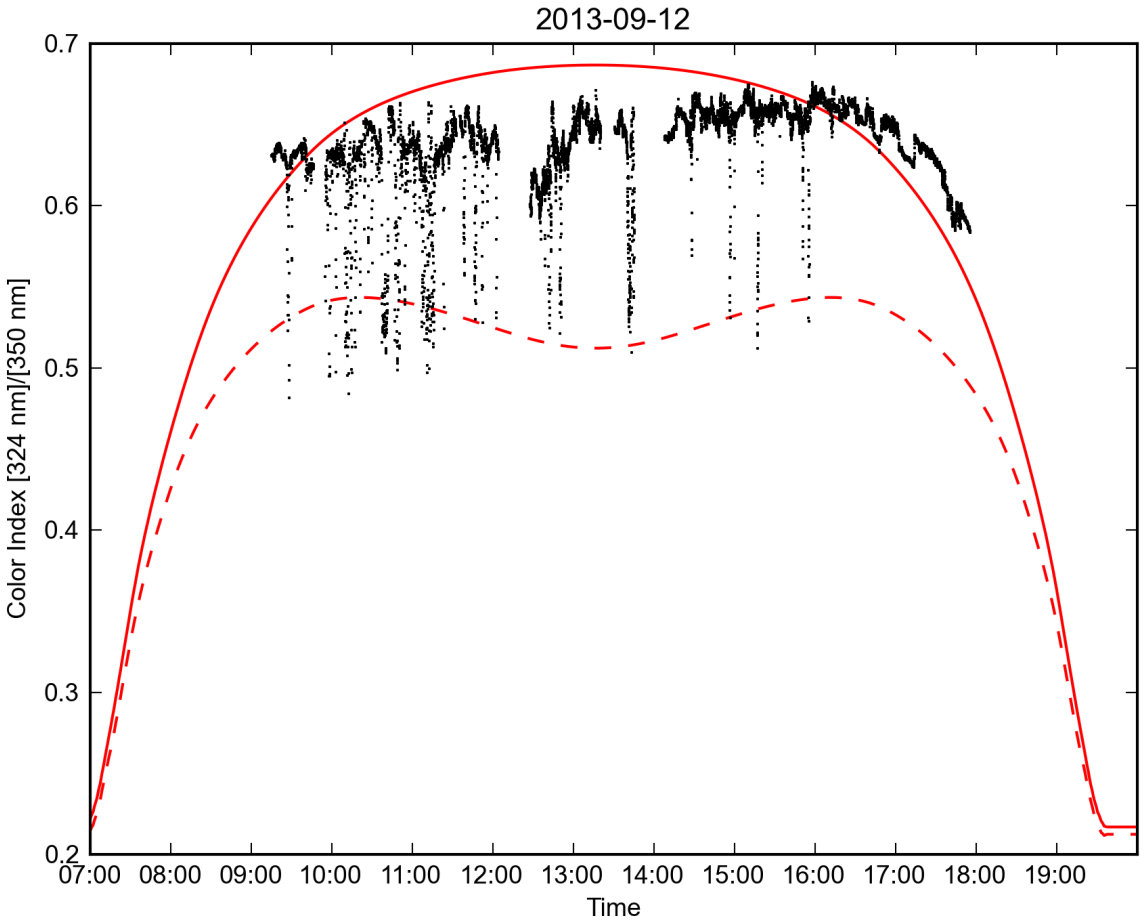
Cloud indicator

Color index $I_{\lambda=324}/I_{\lambda=350}$ for September 25:



Cloud indicator

Color index $I_{\lambda=324}/I_{\lambda=350}$ for September 12:



Cloud indicator

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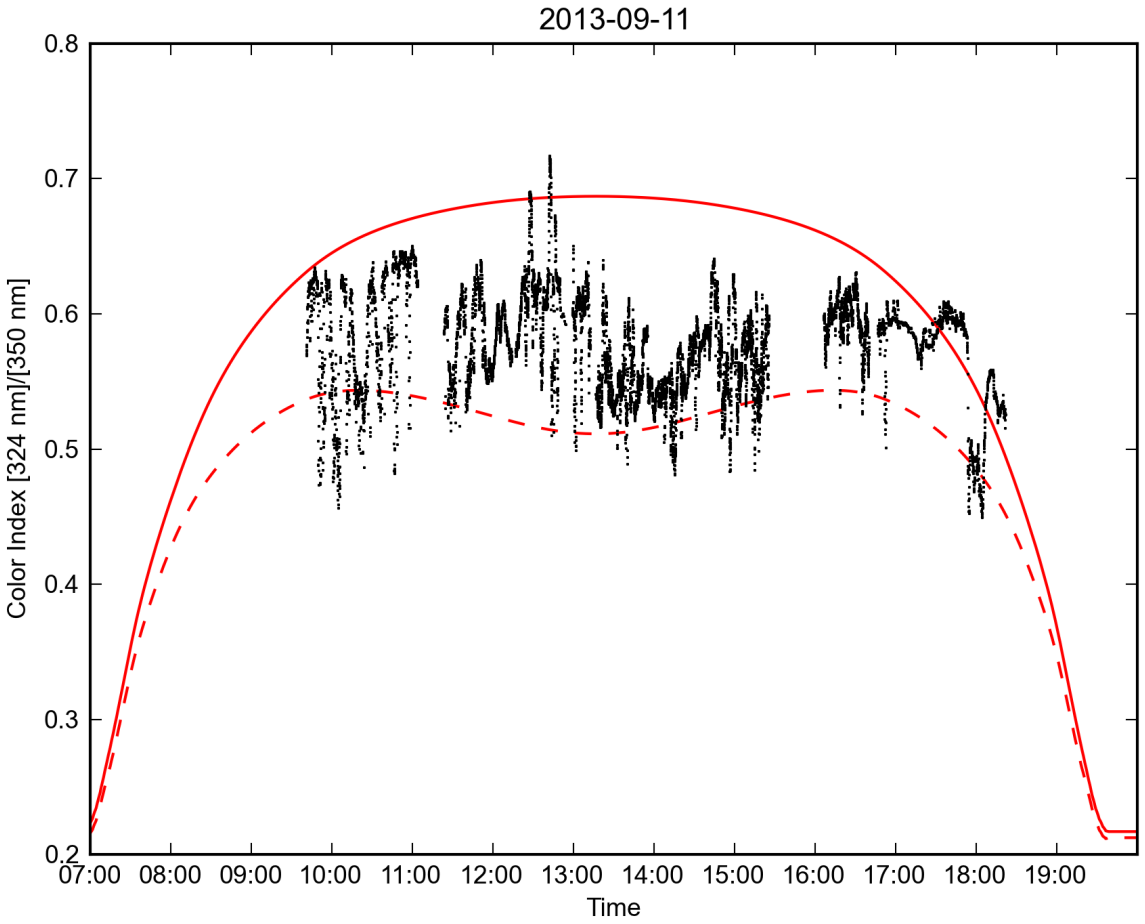
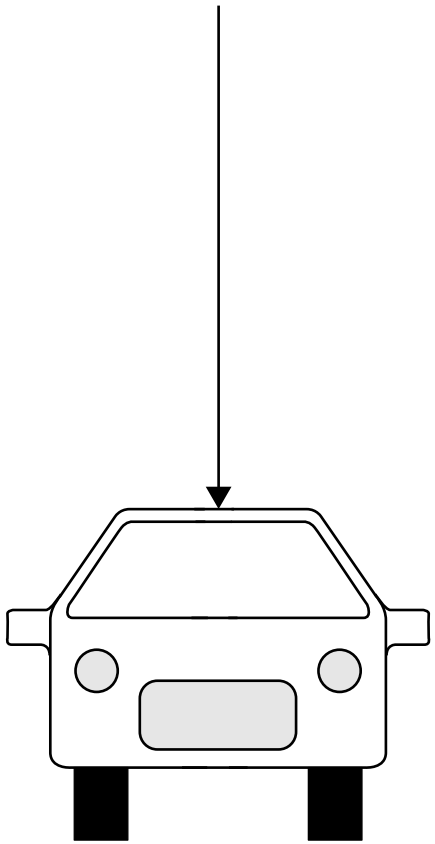


Scanning mode

Experimental mode used at the end of campaign:



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- Use the zenith spectra as reference
- Requires radiative transfer modeling

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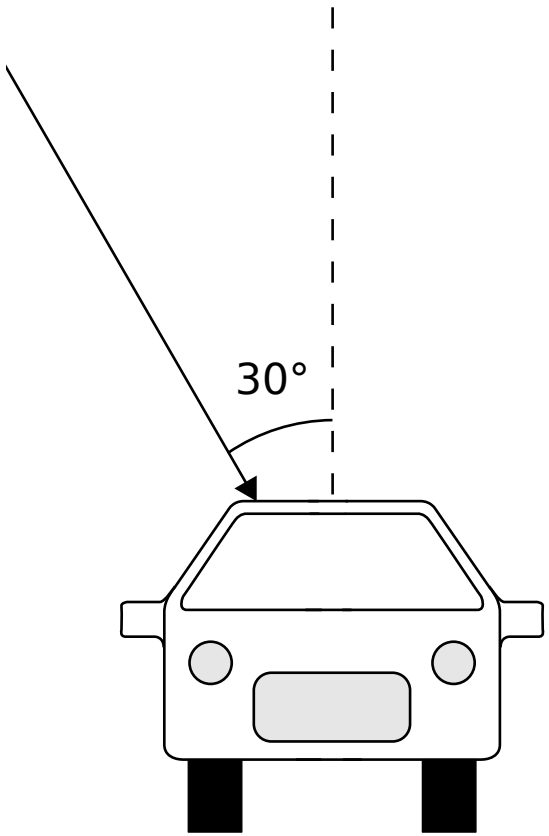

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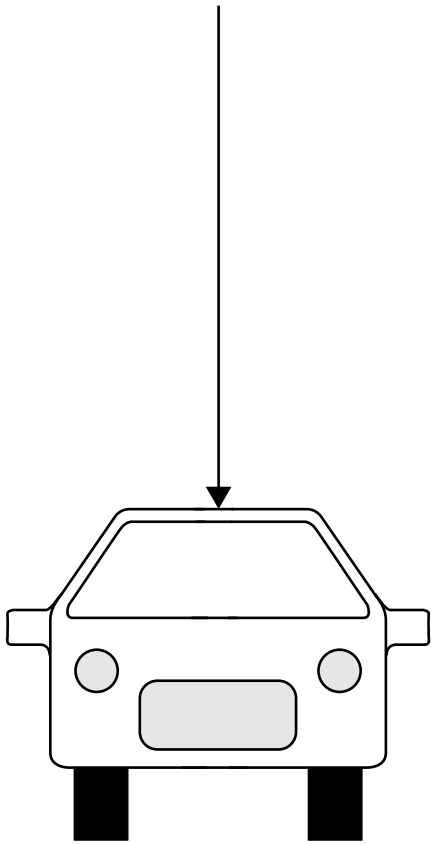

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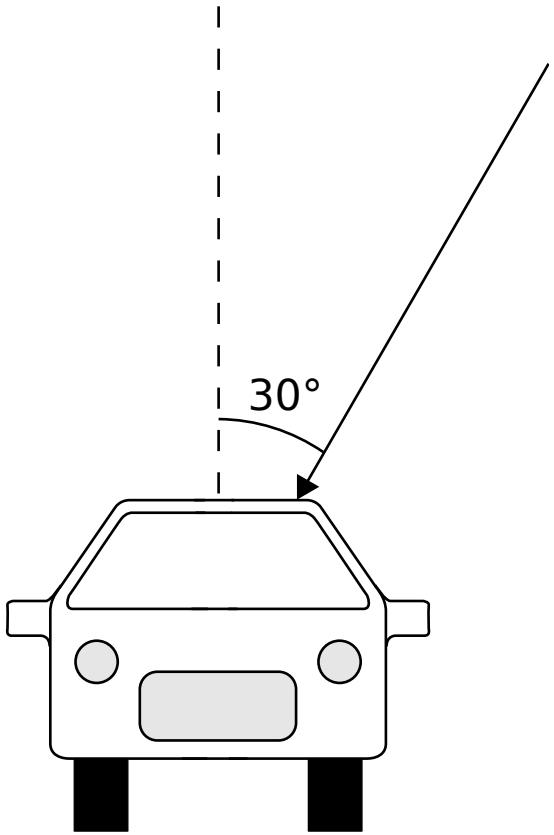

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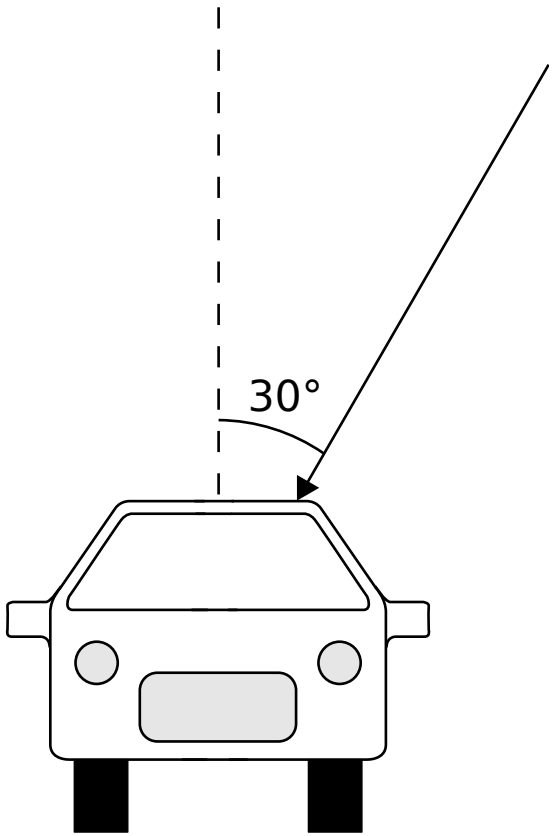

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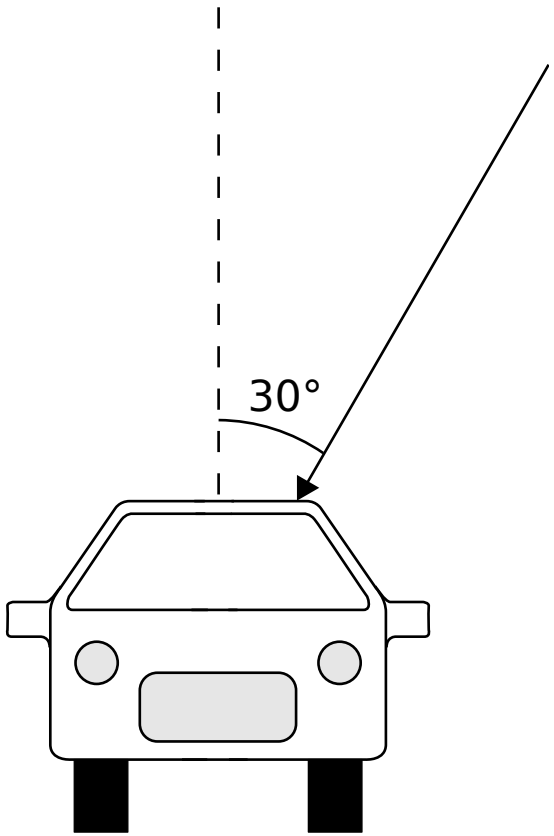

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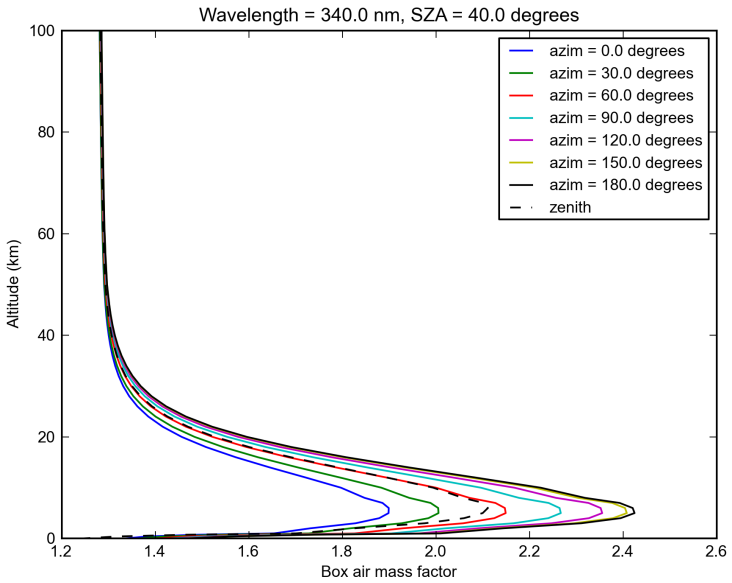
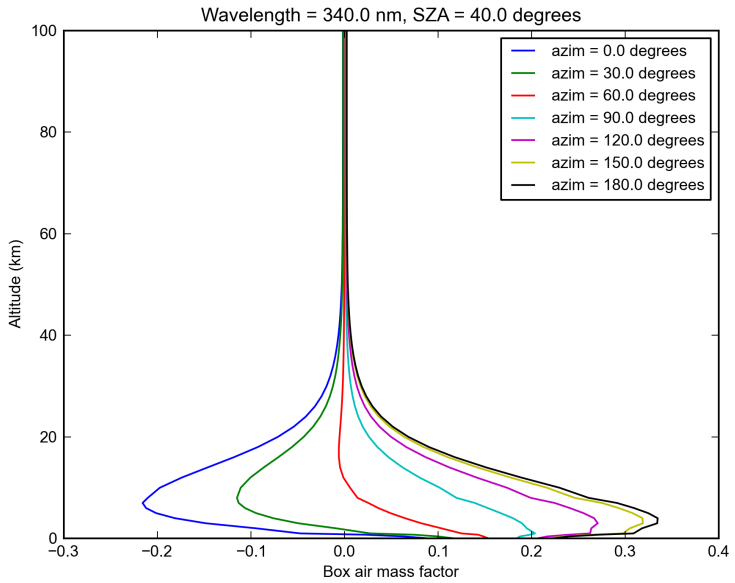
Radiative transfer modeling

Using SCIATRAN model and aerosol profiles measured by aircraft:





Vertical column calculation

Assuming horizontal homogeneity:

$$\Delta\mathrm{SCD} = \int \Delta w(z) n(z) \mathrm{d}z$$

$$\approx \Delta\mathrm{AMF}_{ML} \cdot \mathrm{VCD}_{ML} + \Delta\mathrm{SCD}_{U}$$

Mixing layer column given by:

$$\mathrm{VCD}_{ML} = \frac{1}{\Delta\mathrm{AMF}_{ML}} \left(\Delta\mathrm{SCD} - \Delta\mathrm{SCD}_{U}\right)$$

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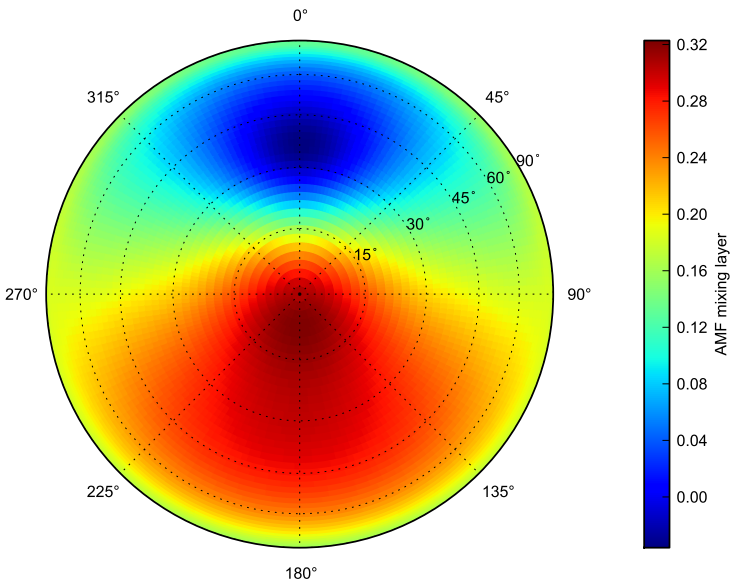
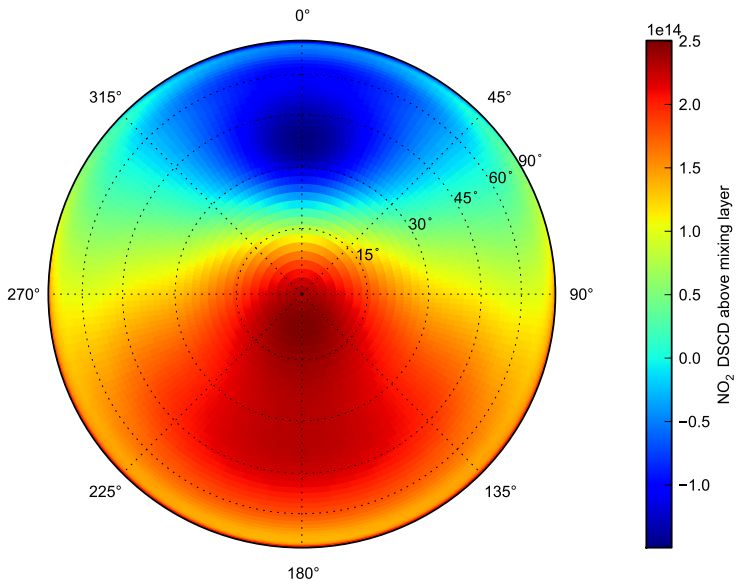
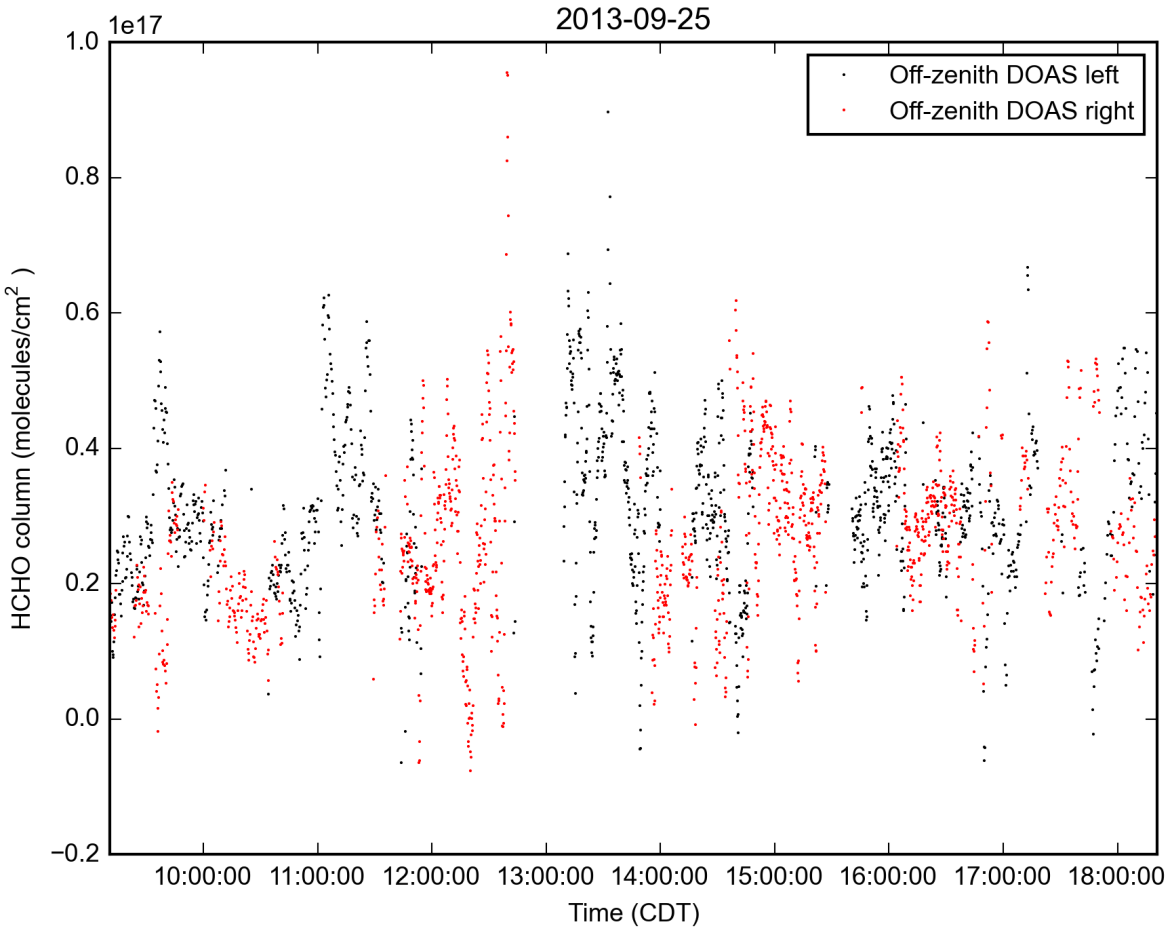
Angular dependence of $\Delta\mathrm{AMF}_{ML}$ and $\Delta\mathrm{SCD}_U$:





Combined approach

Noisy results due to horizontal inhomogeneity. Used to establish an absolute baseline:



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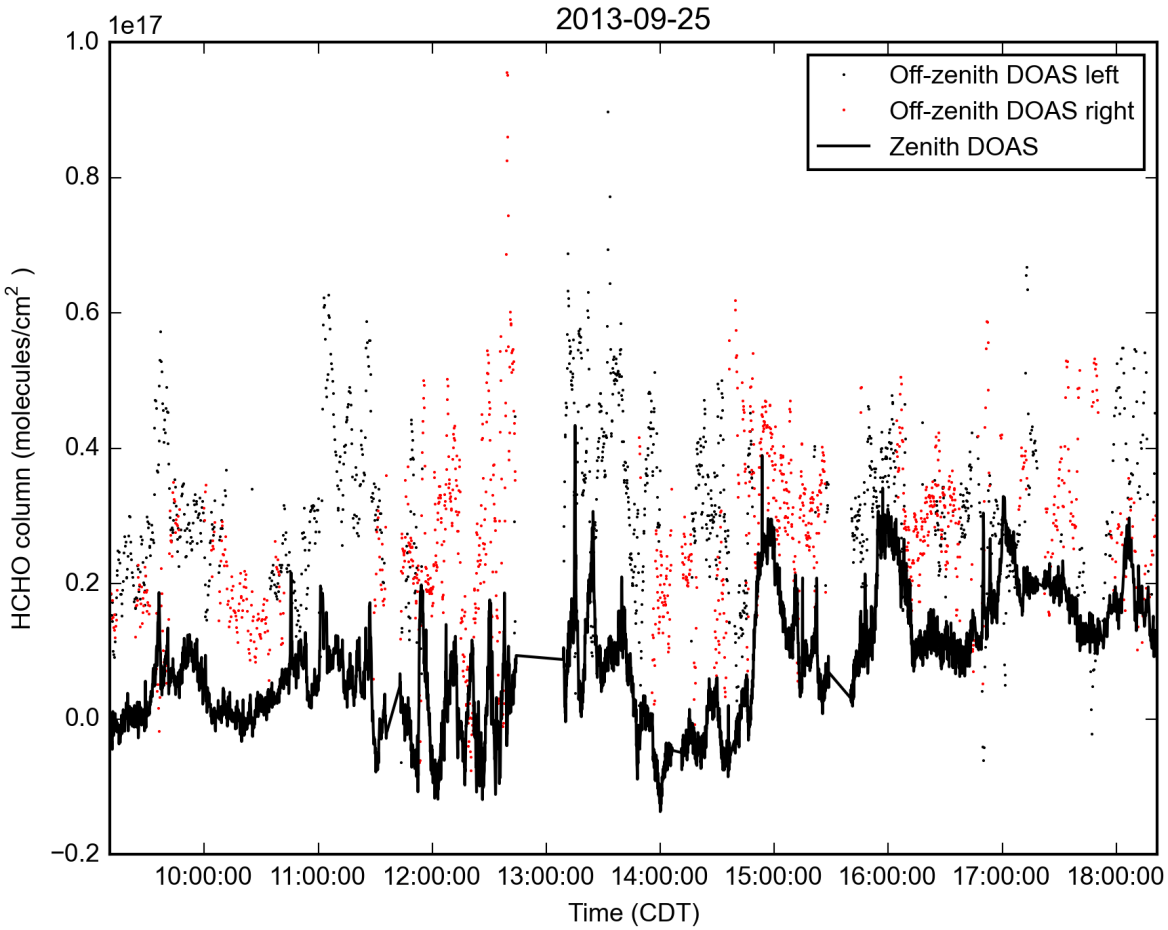

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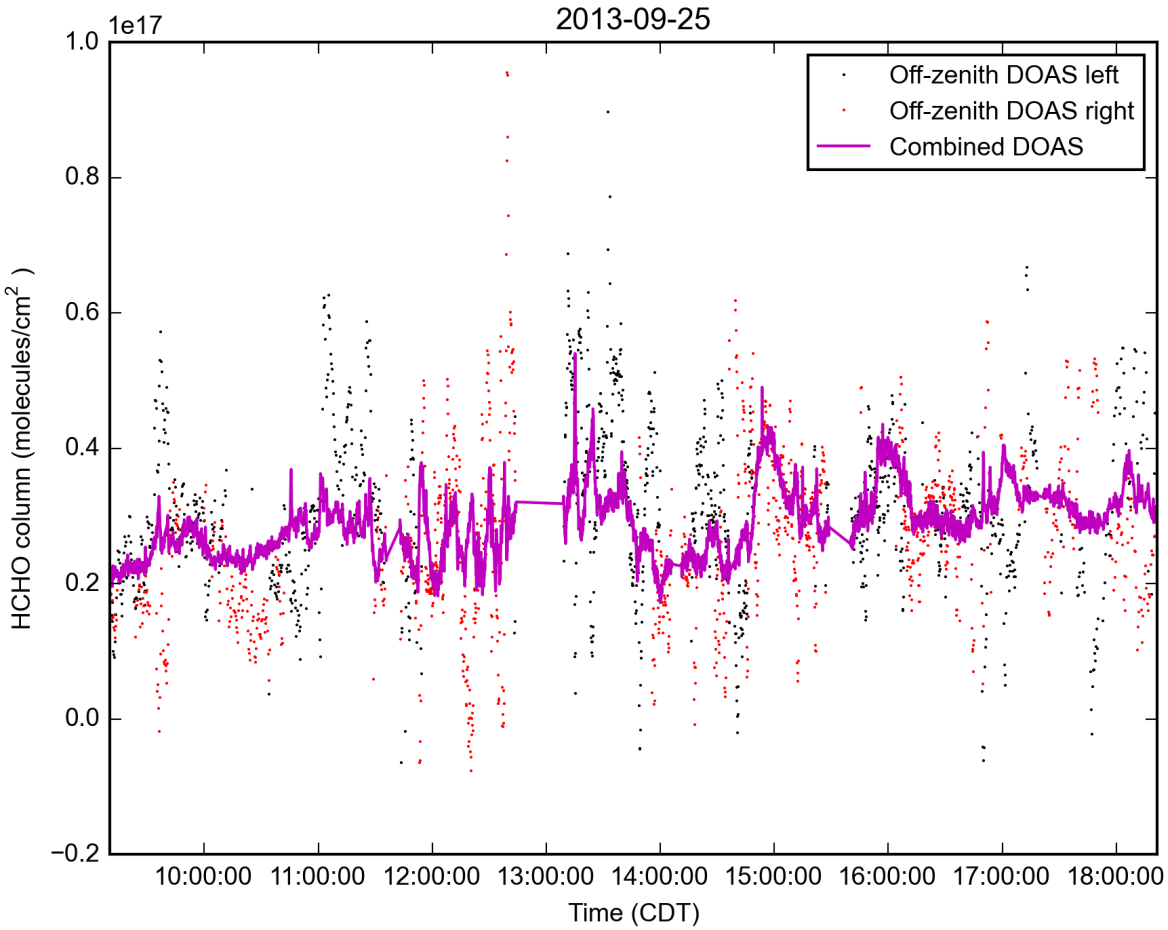

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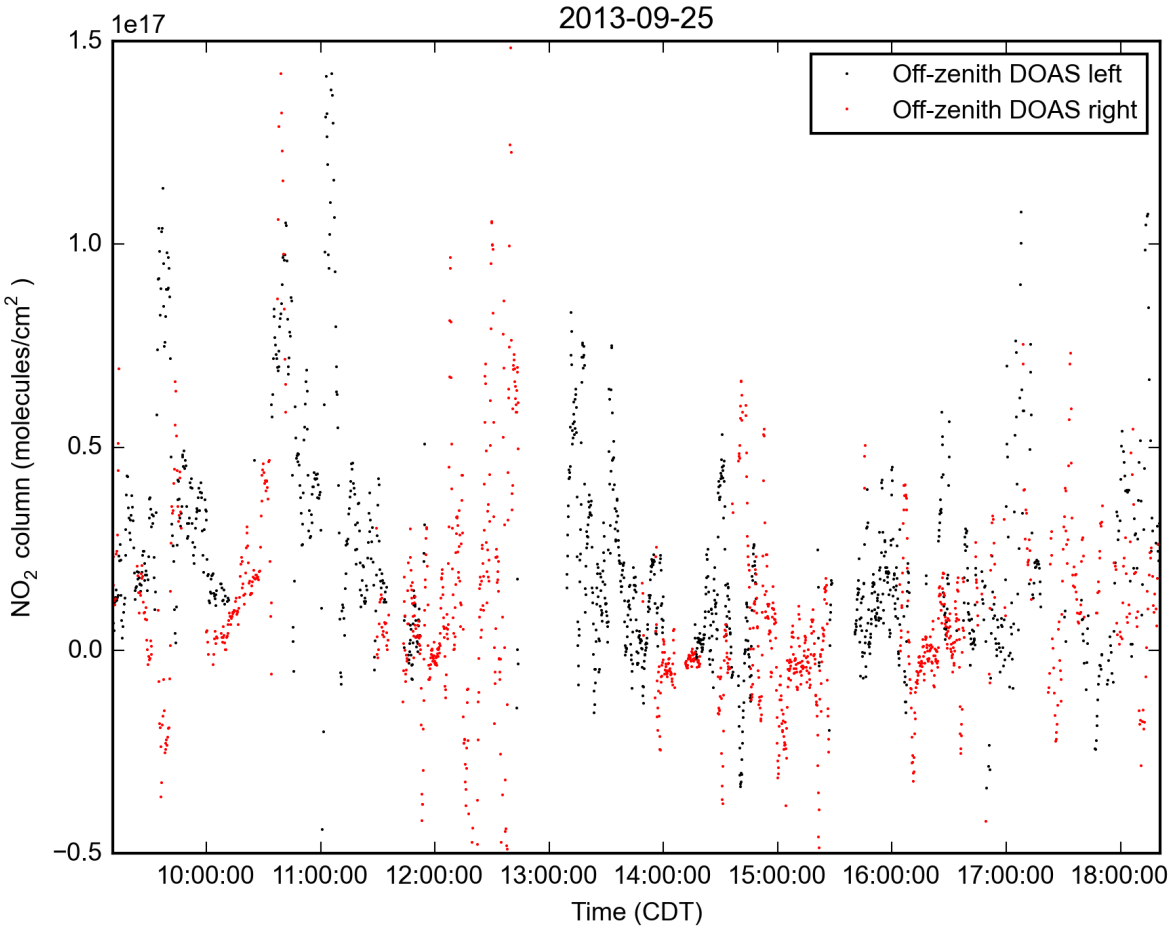
Results for NO_2:



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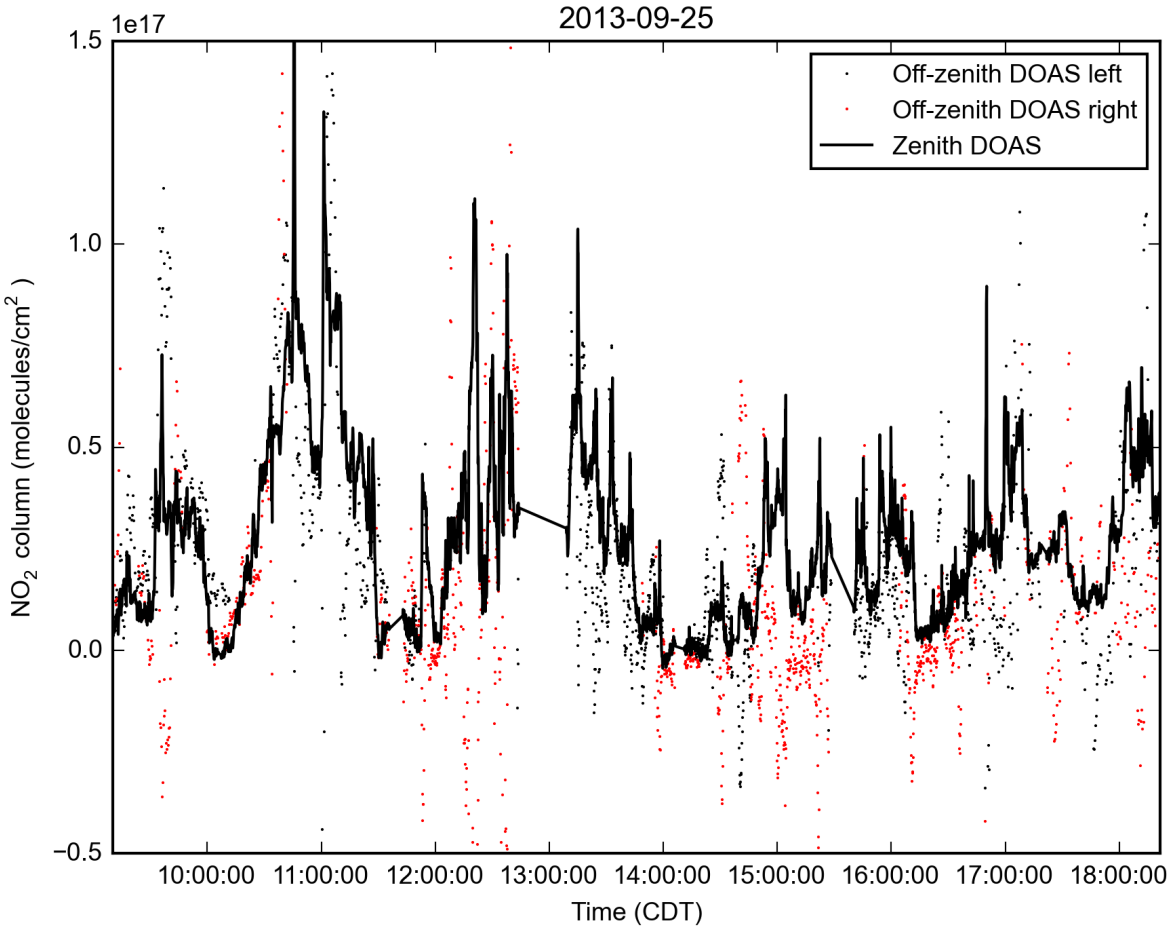

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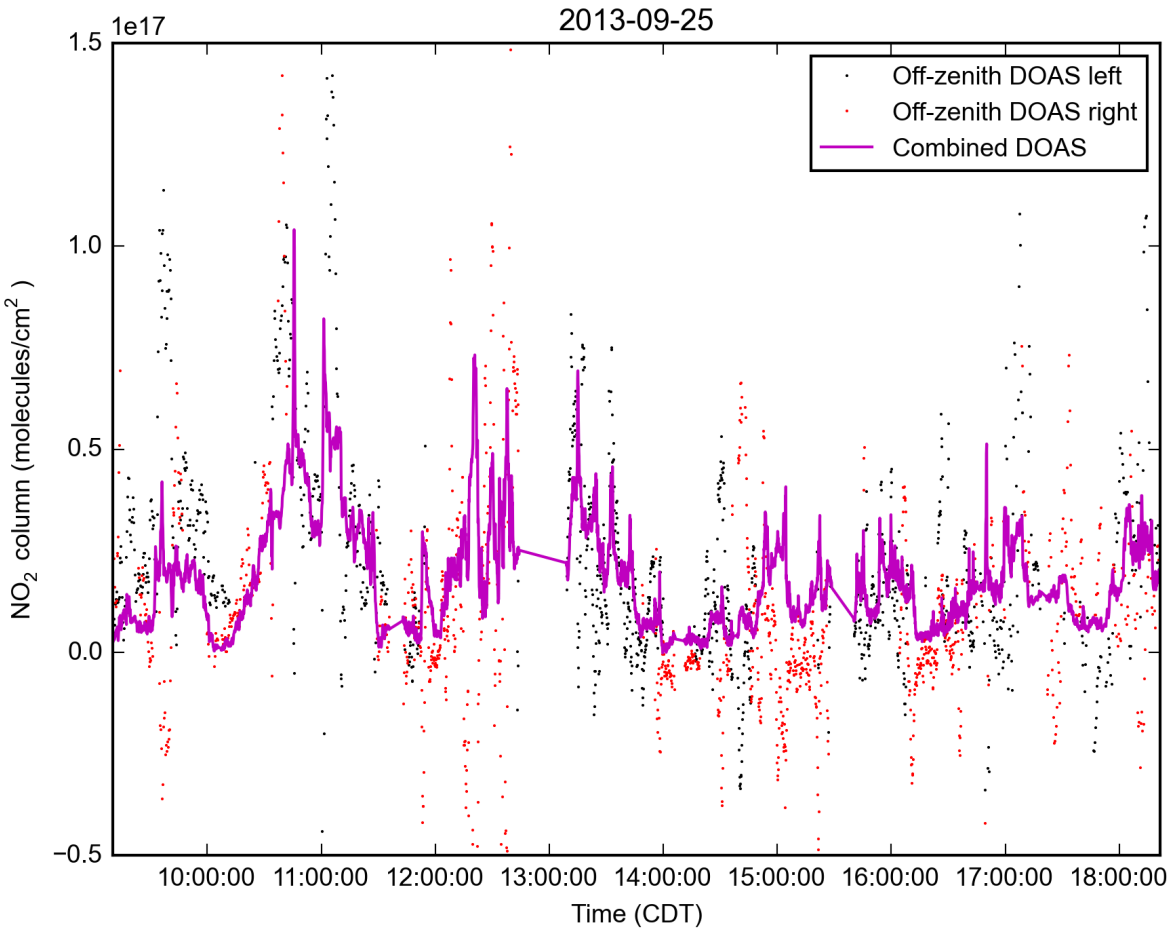
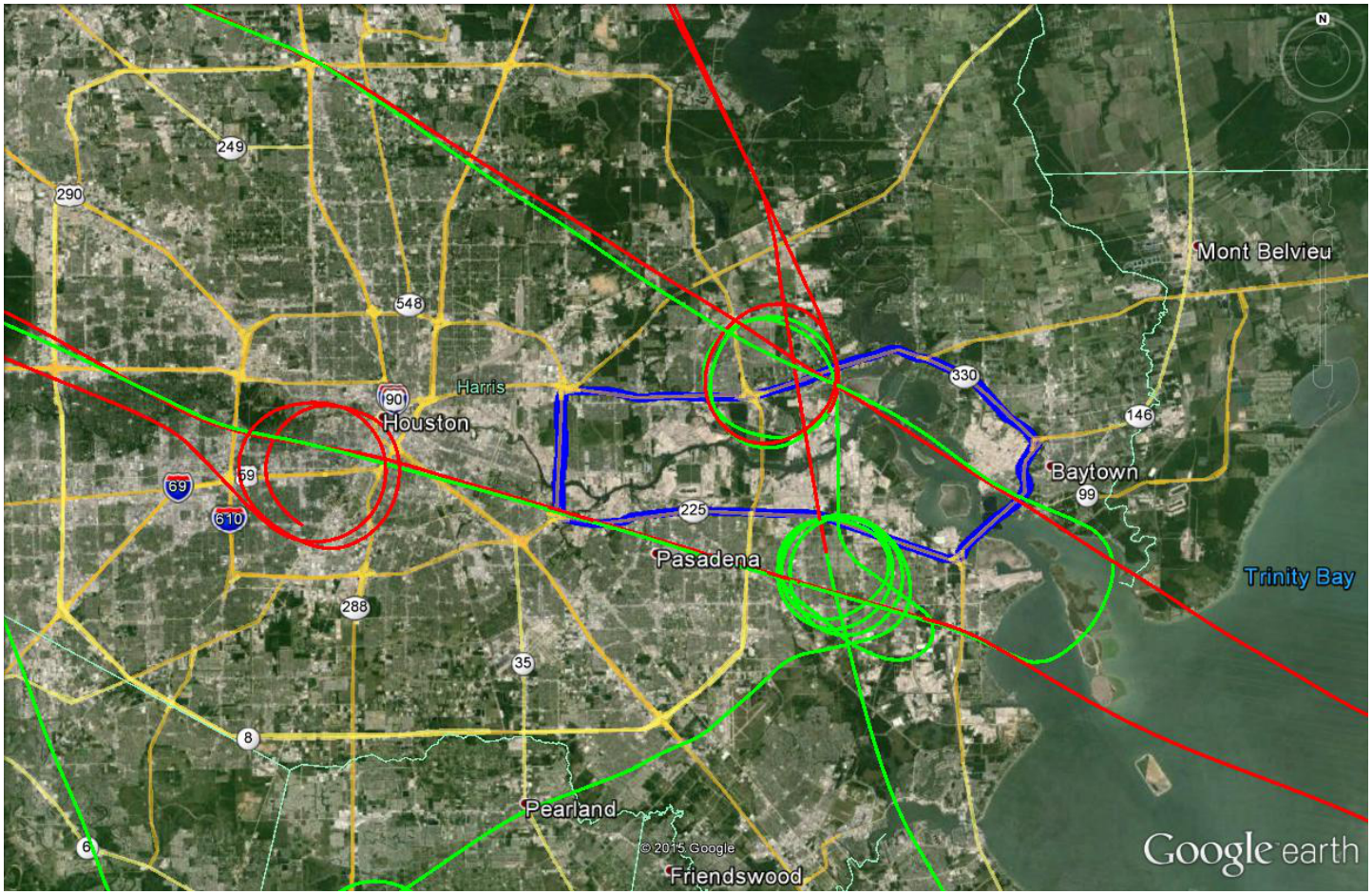


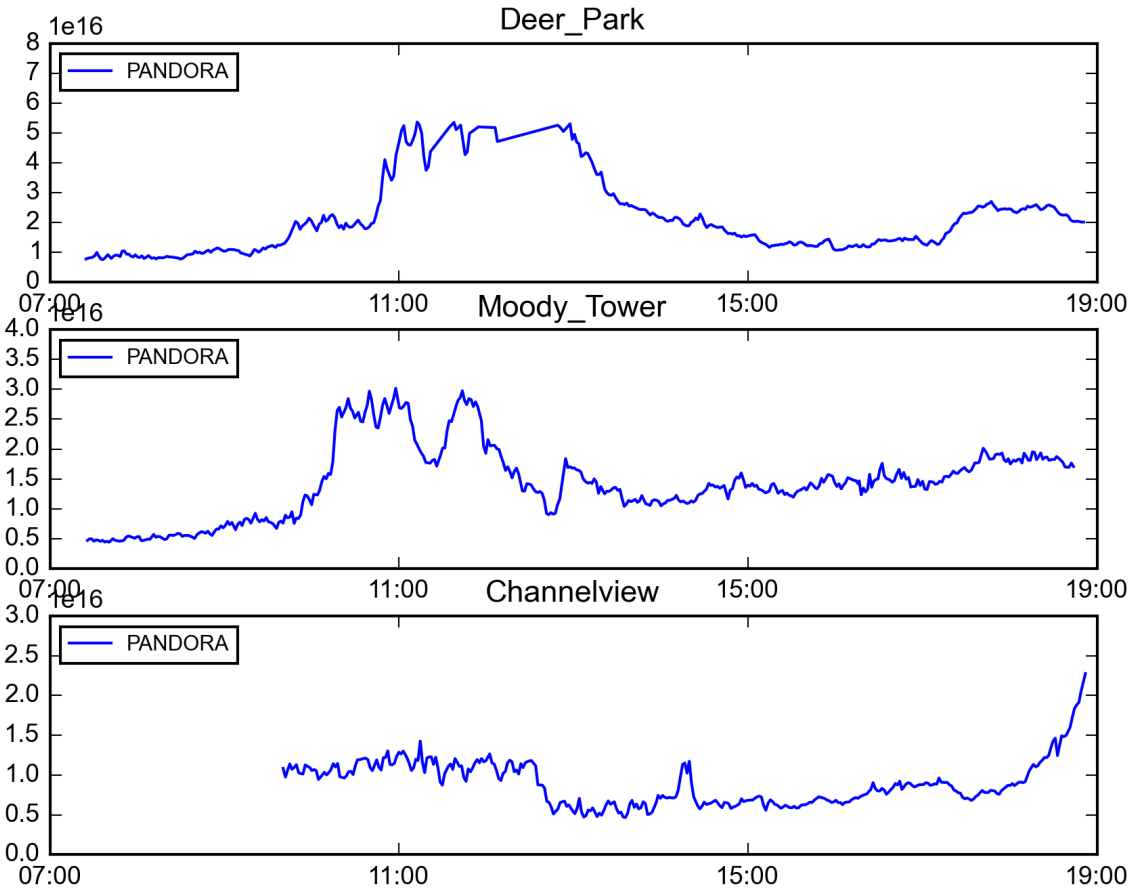
Data comparison

Measurement routes:



Data comparison

Time plots of NO_2 columns at different sites:



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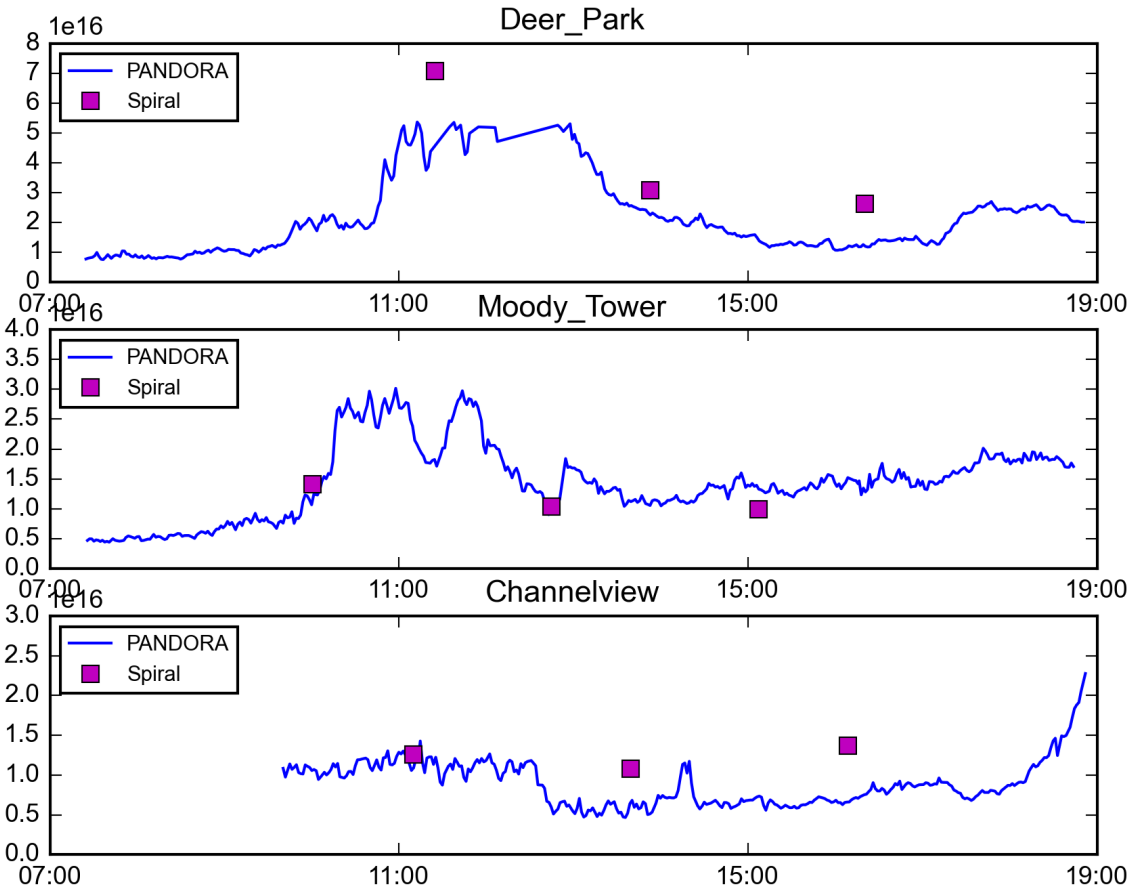

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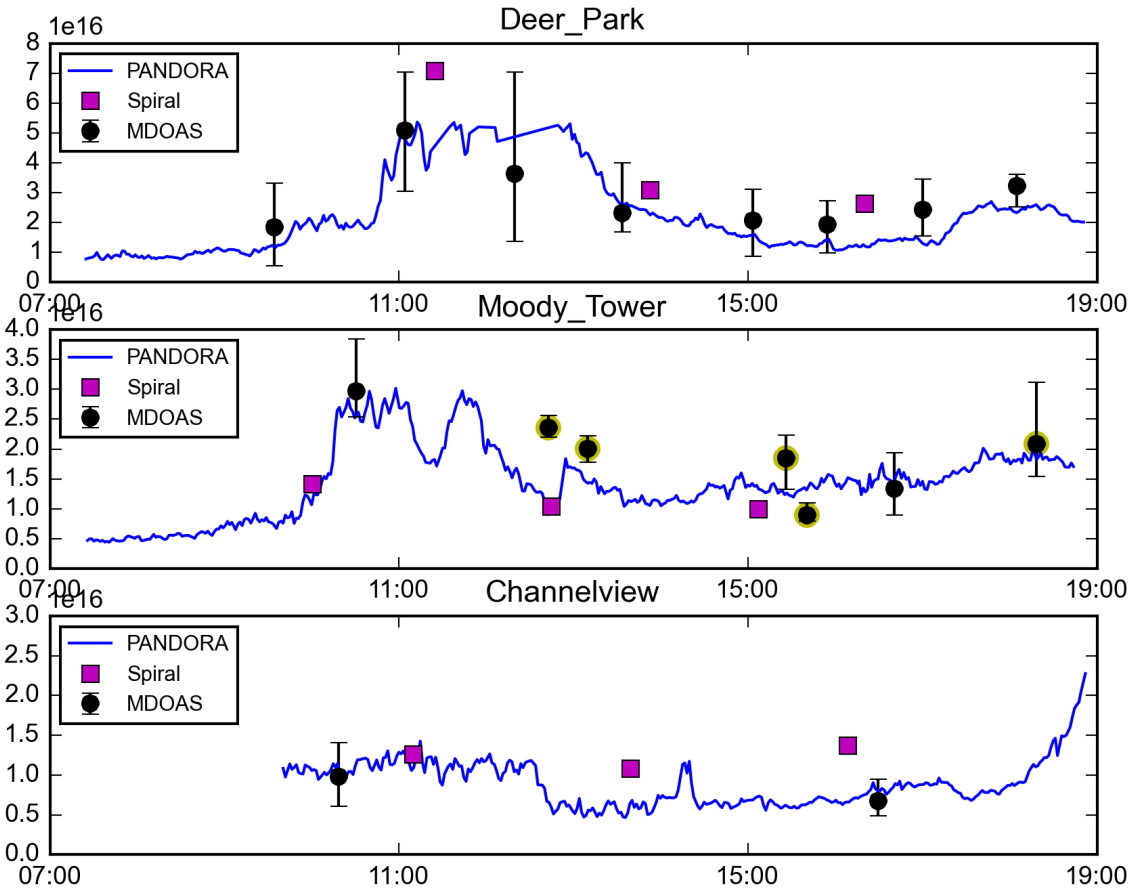

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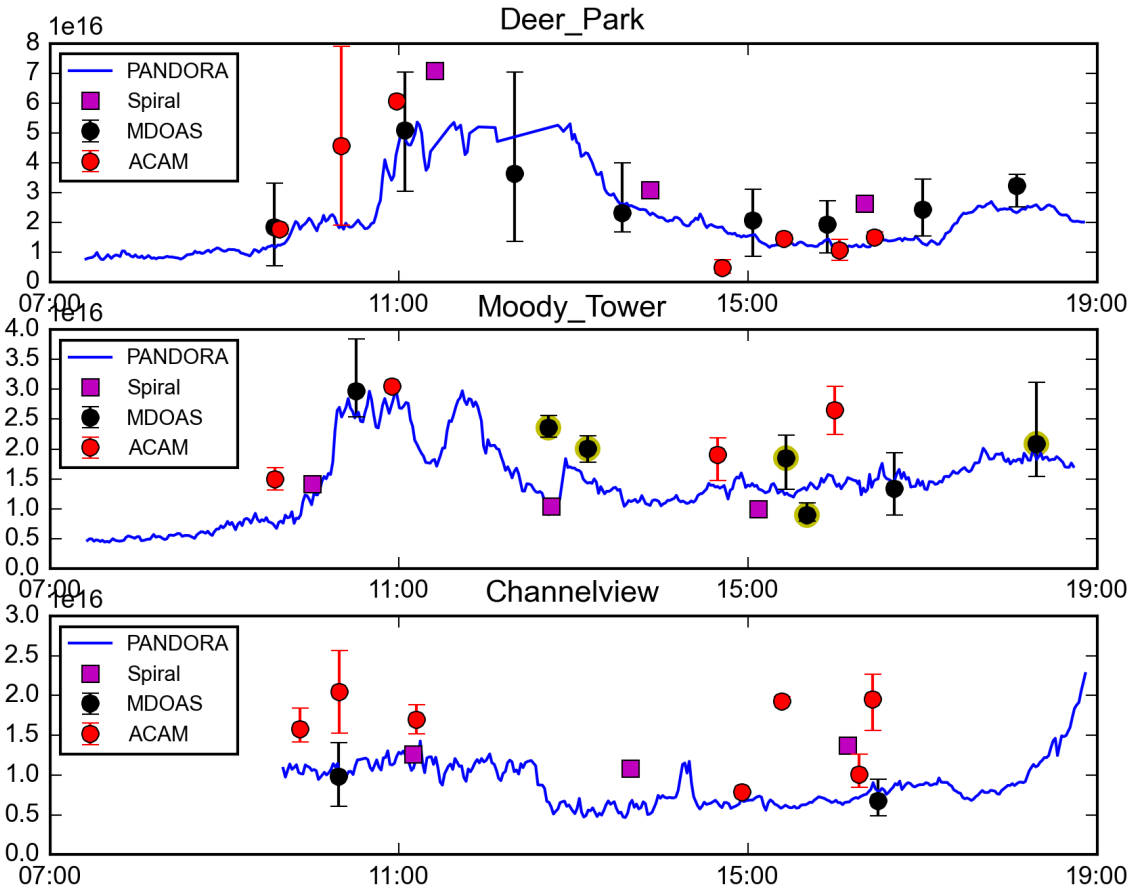
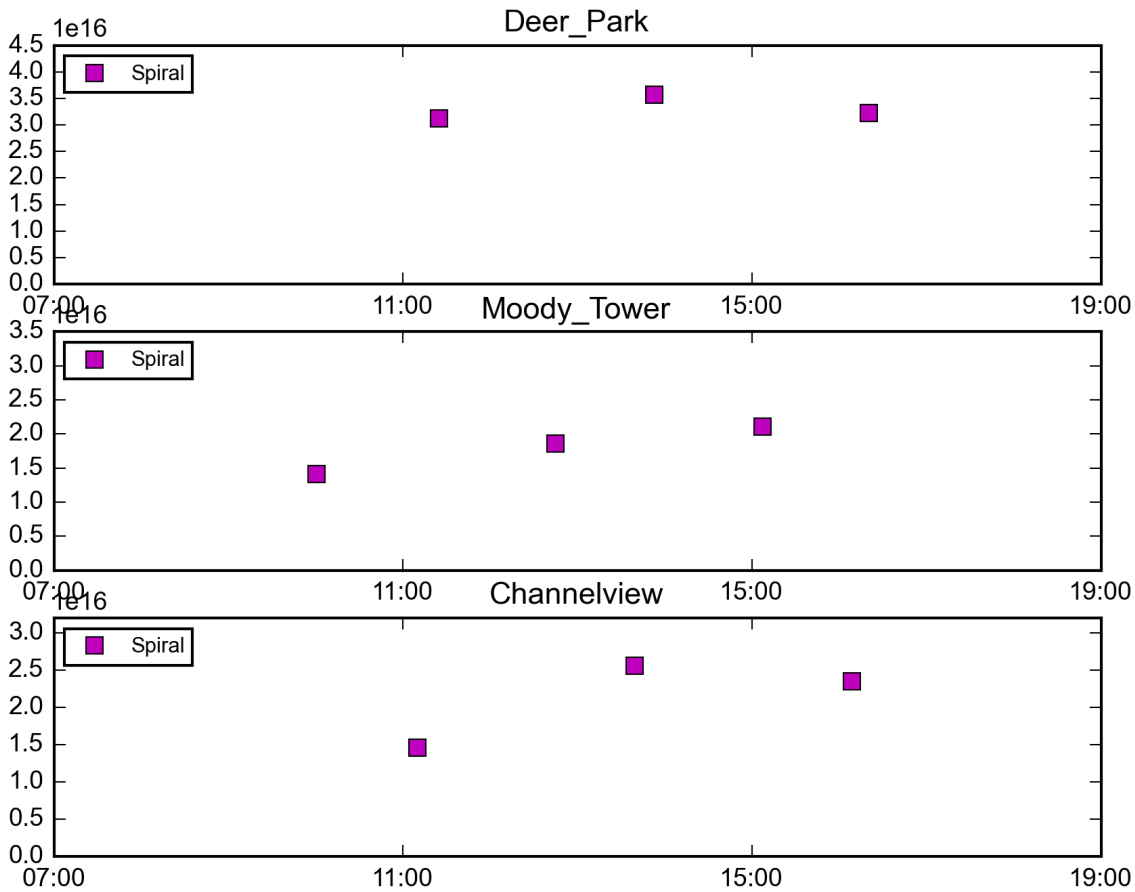


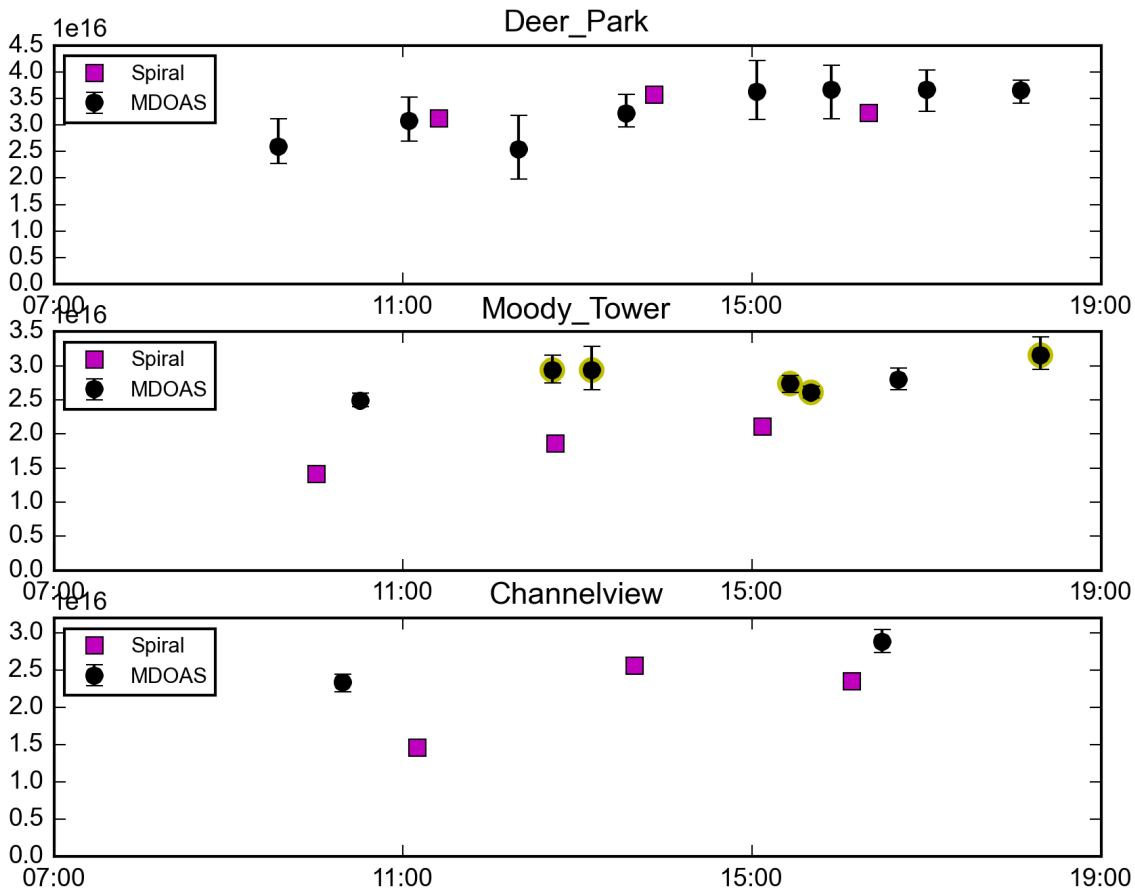
Data comparison

Time plots of HCHO columns at different sites:



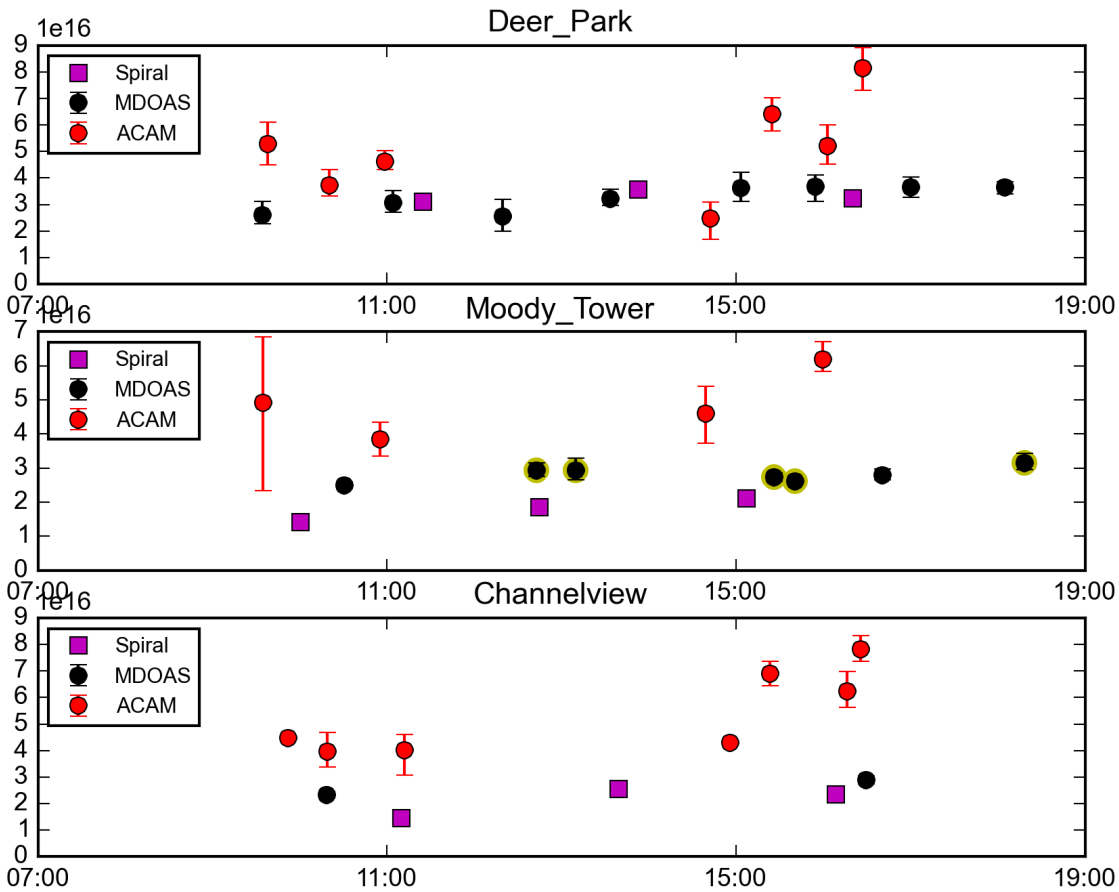
Data comparison

Time plots of HCHO columns at different sites:



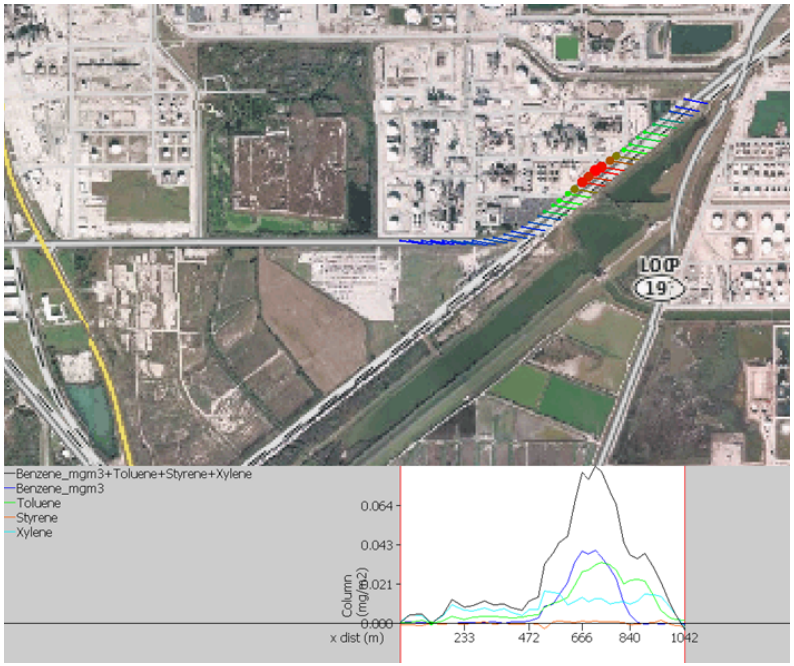
Data comparison

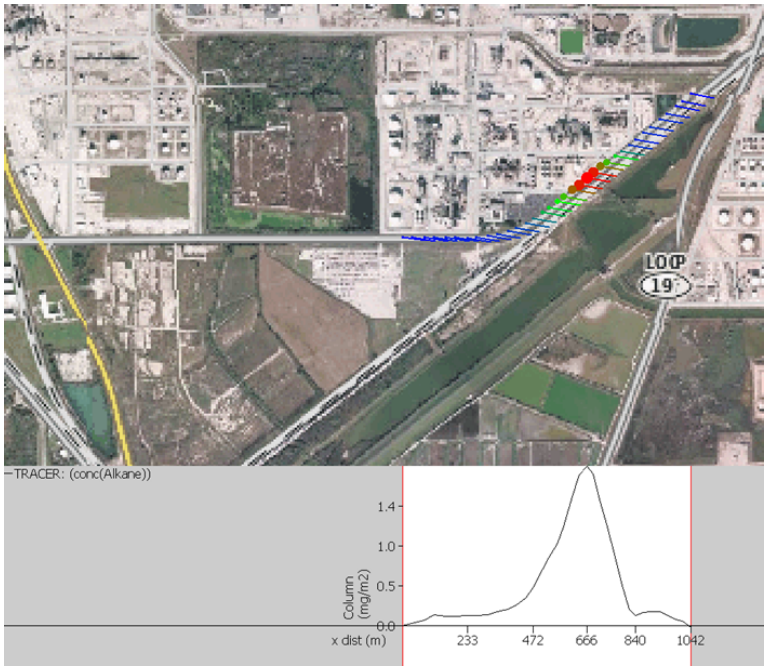
Time plots of HCHO columns at different sites:



MW-DOAS

Measurements of aromatic fraction from Texas City $10 \pm 4\%$:





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