Long-Term comparison of formaldehyde (HCHO) measurements from FTIR and Pandora

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Motivation

❖ Ground-based FTIR and Pandora observations are capable of retrieving similar trace gases, including HCHO, ozone, and NO_2.

❖ Both FTIR and Pandora instruments are well-suited for long-term monitoring, enabling the observation of seasonal patterns and trends over time.

❖ HCHO measurements from FTIR instruments within the Network for the Detection of Atmospheric Composition Change (NDACC; https://ndacc.larc.nasa.gov/) have been widely used for validating low-Earth orbit (LEO) observations, such as TROPOMI (Vigouroux et al., 2020).

❖ While Pandora instruments have demonstrated effective retrieval of NO_2 through direct-sun and multi-axis DOAS observations, HCHO retrieval is more challenging due to its weaker absorption, and limited efforts have focused on validating Pandora HCHO observations (to our knowledge).

❖ While there are numerous Pandora observations within TEMPO's field of regard, only three FTIR sites—Mexico City, Boulder, and Toronto—are available for HCHO comparison. Fortunately, each of these sites has co-located Pandora observations.

PANDONIA (pandoras) and NDACC (HR-FTIR) networks
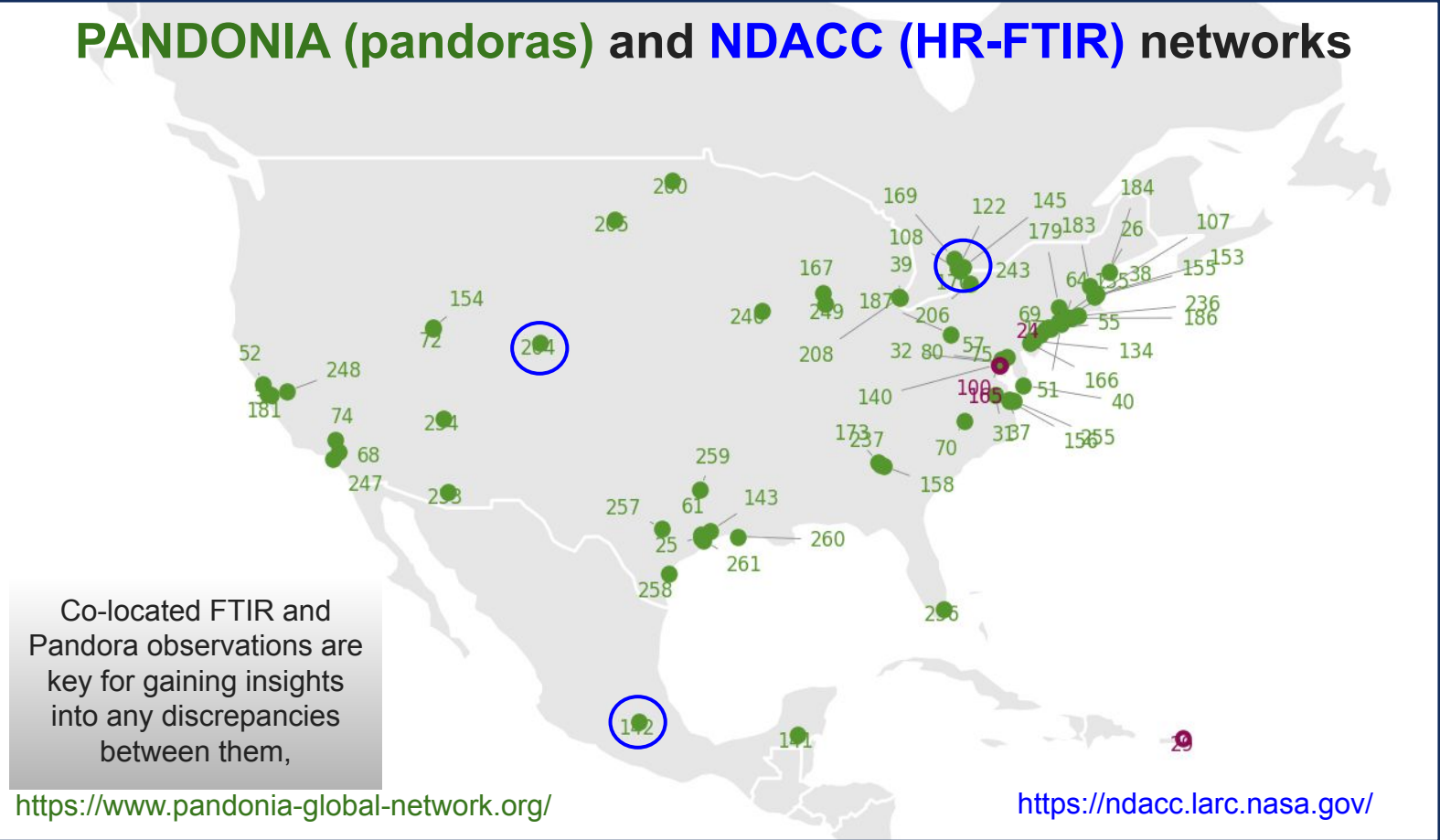
Co-located FTIR and Pandora observations are key for gaining insights into any discrepancies between them,

https://www.pandonia-global-network.org/

https://ndacc.larc.nasa.gov/

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Part 2

Co-located FTIR/Pandora and data products

We use the complete time series of coincident dates available for both Pandora and FTIR.

Observations	Products
FTIR	Direct sun, consolidated and near-real-time analysis following harmonized NDACC retrievals (Vigouroux et al., 2018)
PANDORA	Direct sun; QA L2 flag <=12, tc error <= 30 % Scattered light; QA L2 flag <= 12, error <= 30 %

- For each day with coincident measurements, Pandora observations are interpolated to match the FTIR timestamps. This approach ensures alignment without the need for extrapolation during hours when Pandora data is unavailable.

- For this analysis we focus in trend analysis to see any significant differences. The bias shown in the following slides is defined with the equation below and the reported bias is the median and standard deviation.

$$\text{Bias} = (\text{PANDORA} - \text{FTIR}) / \text{FTIR}$$

Boulder: Total Columns

All data
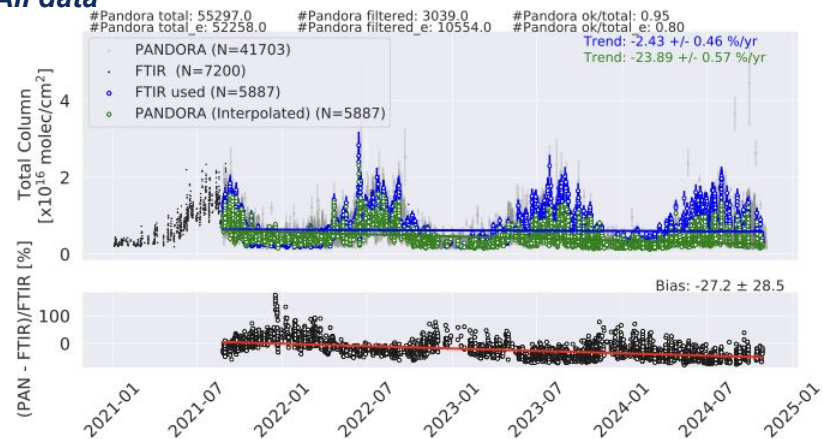
Monthly

Long-term trend and the seasonal modulation

$$f(t) = a_0 + a_1(t - t_0) + \sum_{n=1}^{N} b_n \cos\left(\frac{n\pi x}{L}\right) + \sum_{n=1}^{N} c_n \sin\left(\frac{n\pi x}{L}\right)$$

Linear component

Fourier series

Instrument	Trend [%/y]	Bias [%]
FTIR	-2.43 ± 0.46	-27.2 ± 28.5
Pandora	-23.89 ± 0.57	

Some comments:

- Clearly the trends between FTIR and Pandora are different.

- Clear negative trend in the bias.
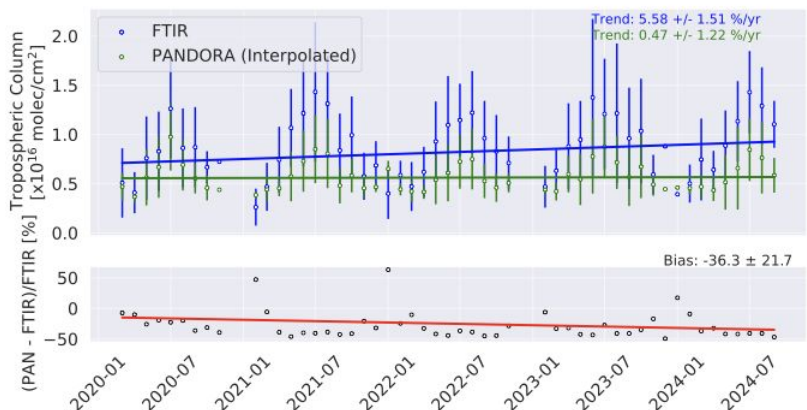
Boulder: Tropospheric columns

All data
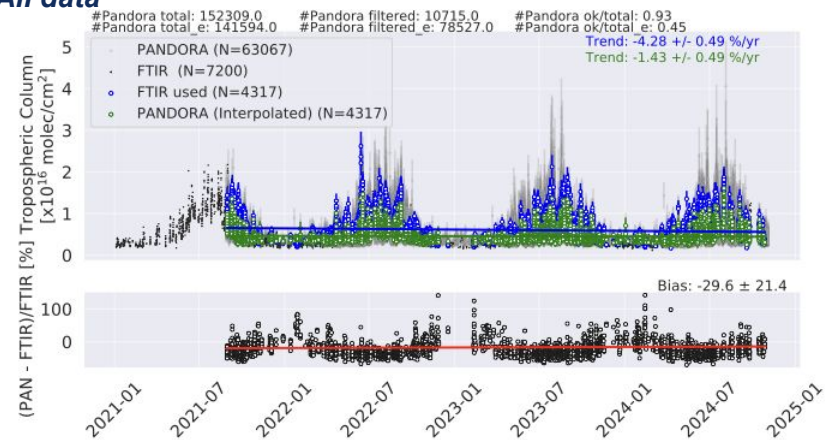
Monthly

Instrument	Trend [%/y]	Bias [%]
FTIR	-4.28 ± 0.49	-29.6 ± 21.4
Pandora	-1.43 ± 0.49	

Some comments:

- Trends between FTIR and Pandora are similar.

- Seasonal bias is identified. Lower and/or positive bias is captured in some winter months.
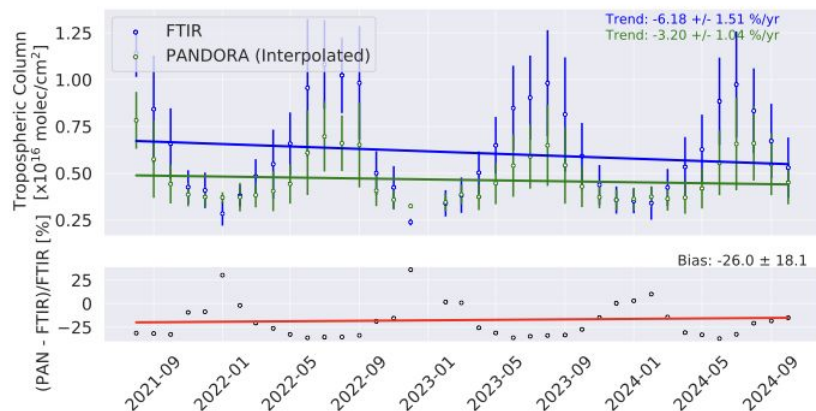
Toronto: Total Columns

All data
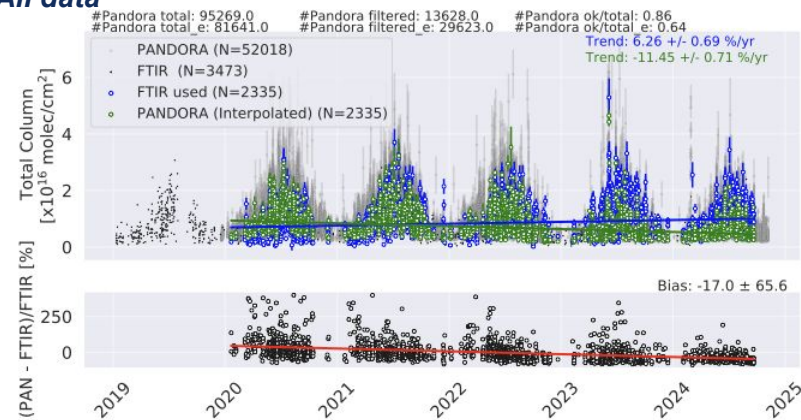
Monthly

Instrument	Trend [%/y]	Bias [%]
FTIR	+6.26 ± 0.69	-17.0 ± 65.6
Pandora	-11.45 ± 0.71	

Some comments:

- Clearly the trends between FTIR and Pandora are different.

- Clear negative trend in the bias.
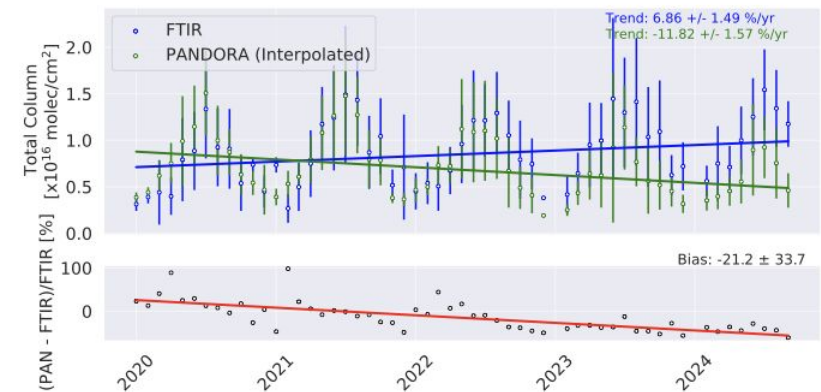
Toronto: Tropospheric columns
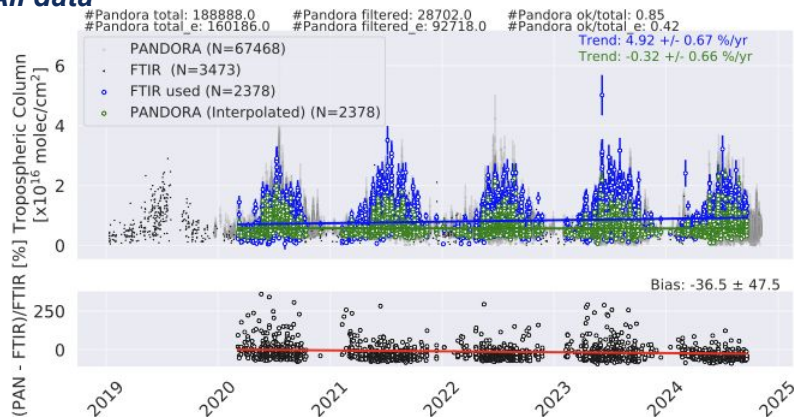
All data

Monthly

Instrument	Trend [%/y]	Bias [%]
FTIR	+4.92 ± 0.67	-36.3 ± 21.7
Pandora	-0.32 ± 0.66	

Some comments:

- Trends between FTIR and Pandora are not very different.

- SLower and/or positive bias is captured in some winter months.

Mexico City: Total Columns

All data
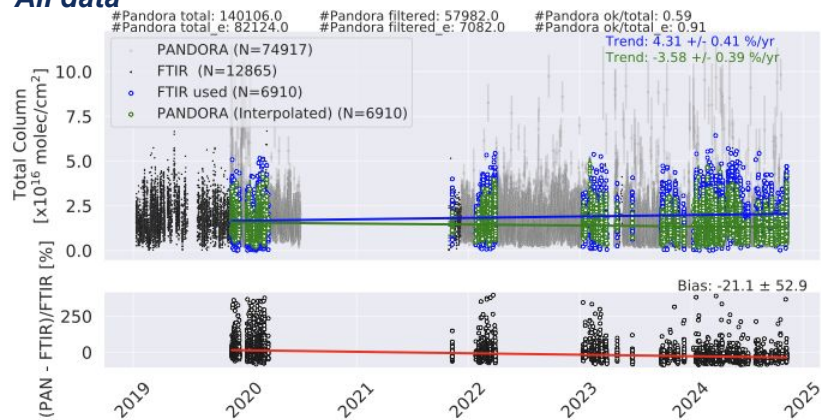
Monthly

Instrument	Trend [%/y]	Bias [%]
FTIR	+4.31 ± 0.41	-21.1 ± 52.9
Pandora	-3.58 ± 0.39	

Some comments:

- Clearly the trends between FTIR and Pandora are different.

- Clear negative trend in the bias.

- Initial months show similar columns then the comparison degrades.
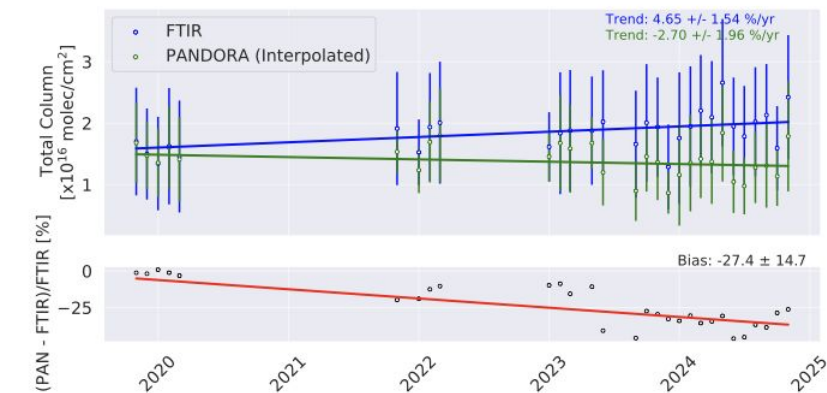
Mexico City: Tropospheric columns

All data
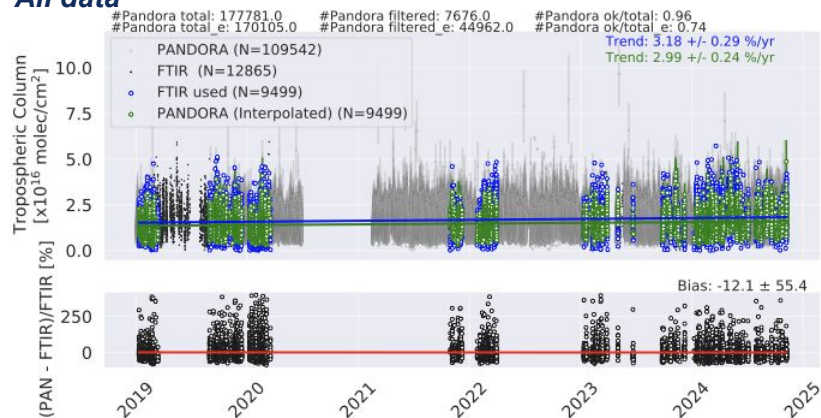
Monthly

Instrument	Trend [%/y]	Bias [%]
FTIR	**+3.18 ± 0.29**	-12.1 ± 55.4
Pandora	+2.99 ± 0.24	

Some comments:

- Trends between FTIR and Pandora are very similar.

- Low bias
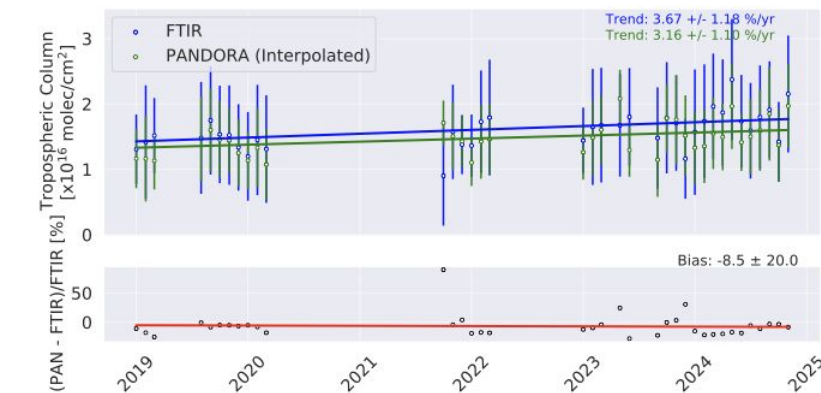
Summary/Conclusions

- The trends in Pandora total columns show poor alignment with those observed in FTIR total columns. Additionally, further analysis reveals that these trends also diverge from the tropospheric FTIR and Pandora column trends.

- The comparison between FTIR and Pandora total columns initially shows good agreement after Pandora installation, but over time, a negative trend develops in the Pandora total columns, leading to a degradation in bias.

- A few months ago Luke Valin shared with me about this issue where he has seen "*systematic residuals grow over time*"

- What could be driving this negative trend? Could it be linked to the reference HCHO used in the analysis, stray light, stability of spectrometer, or another factor(s)?.

- What about other sites?

- What does this mean for TEMPO comparisons? → May be site dependent and need to check when Pandora was installed. I would recommend using tropospheric columns unless total columns are corrected.

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The middle panels in the plots below show the de-seasonal columns for both FTIR and Pandora. The de-seasonal values have been estimated using the observed columns minus the Fourier series (without trends). The slopes, in molec/cm^2 per year are included in the middle panels.
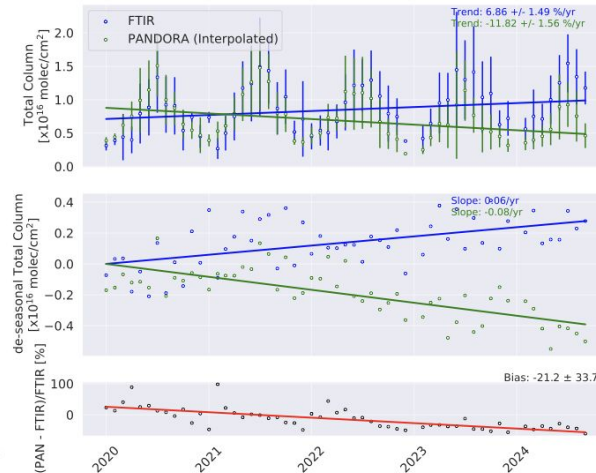
Total Columns
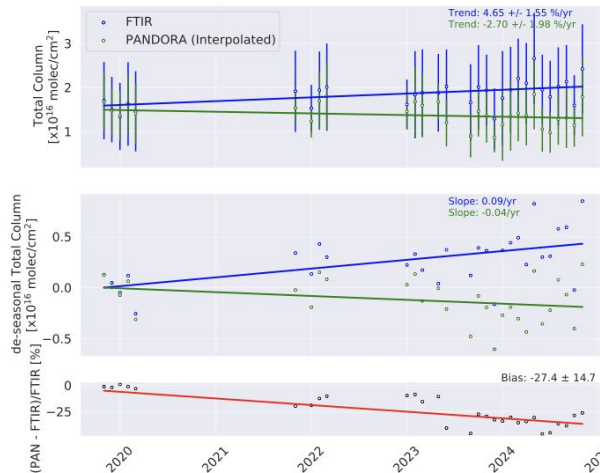
Total column trends between FTIR and Pandora do not agree - similar results

Does performing a de-seasonal analysis significantly impact the observed trends?

The middle panels in the plots below show the de-seasonal columns for both FTIR and Pandora. The de-seasonal values have been estimated using the observed columns minus the Fourier series (without trends). The slopes, in molec/cm^2 per year are included in the middle panels.

Tropospheric Columns
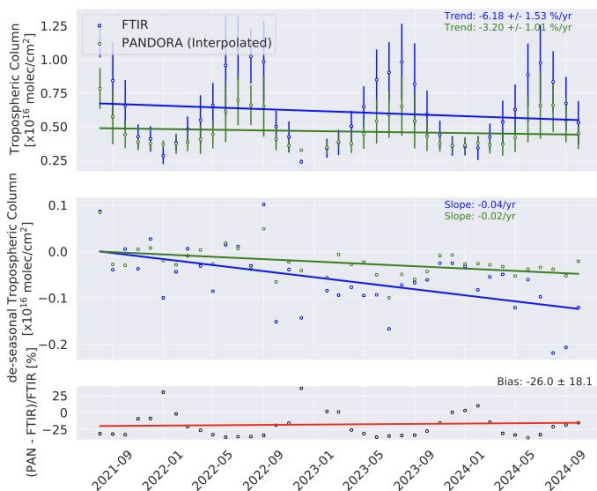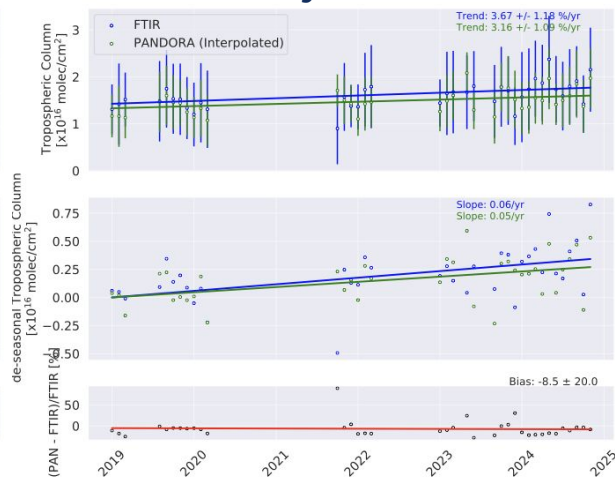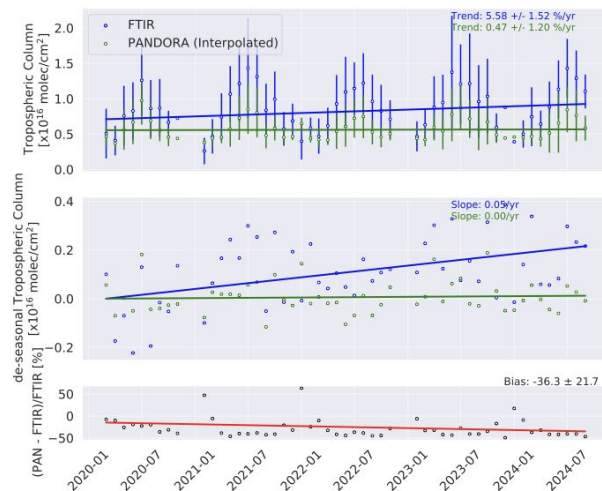
Tropospheric column trends between FTIR and Pandora agree well

Ground-based FTIR and Pandora can retrieve similar gases like HCHO, Ozone, and NO$_2$. FTIR has been used to validate HCHO measurements with TROPOMI (Vigouroux et al., 2020).
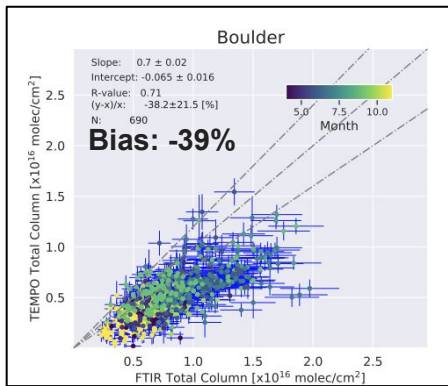
*Example of TEMPO L2 V3 HCHO on Aug 11 2023*
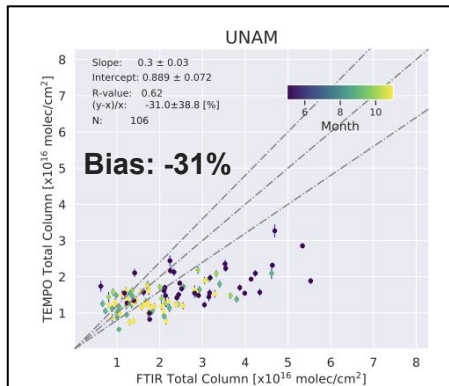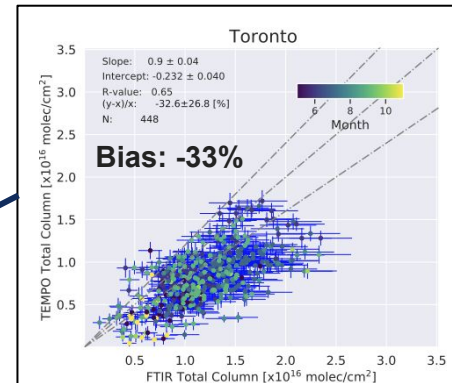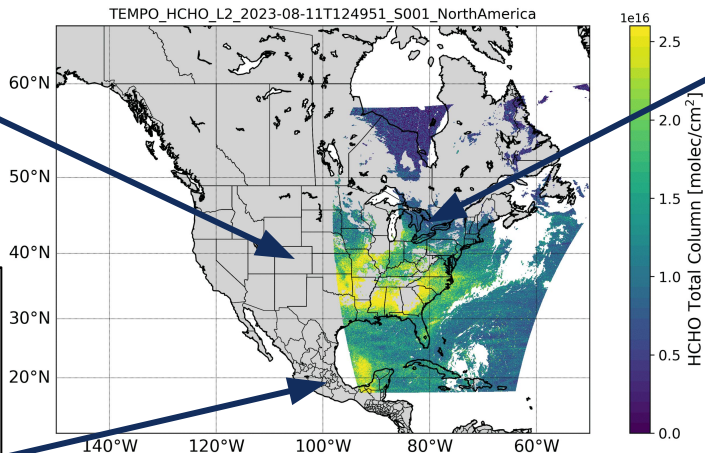
Data from Aug 2023 - Oct 2024

Bias = (TEMPO-FTIR)/FTIR

- Strong and consistent correlation between TEMPO and FTIR → extremely encouraging results!

- TEMPO HCHO total columns observations are about 30 % lower than FTIR.

Could the underestimation be attributed to the radiance reference in TEMPO?
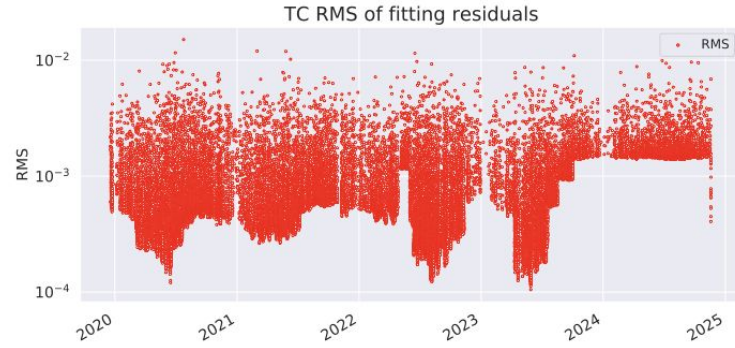
Direct sun; QA L2 flag <=12, tc error <= 50 %

Boulder
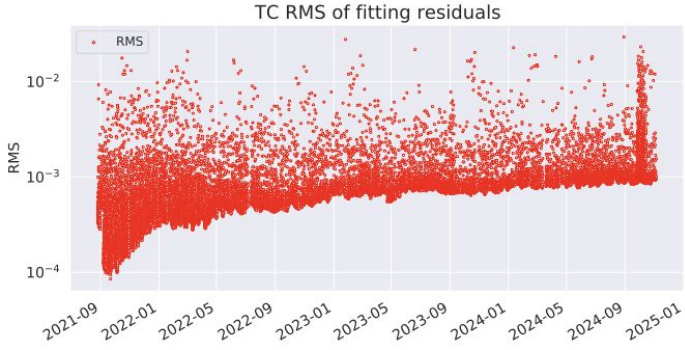
Toronto

Mexico City
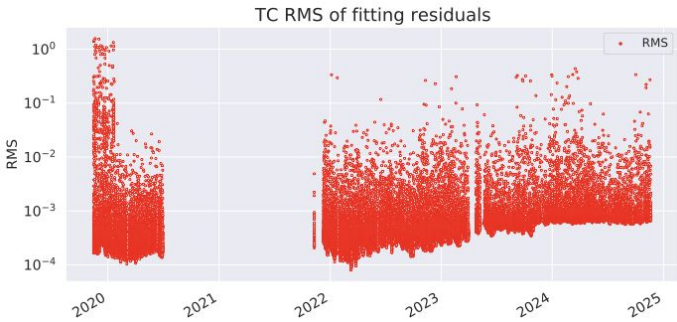
After recently downloading the Pandora data and conducting the same analysis, the significant negative linear trend has disappeared in the Pandora - leading to improved agreement with the FTIR measurements.
From Tom: A correction in the drift in the wavelength resolution in the spectrometer has been applied using a new field calibration.

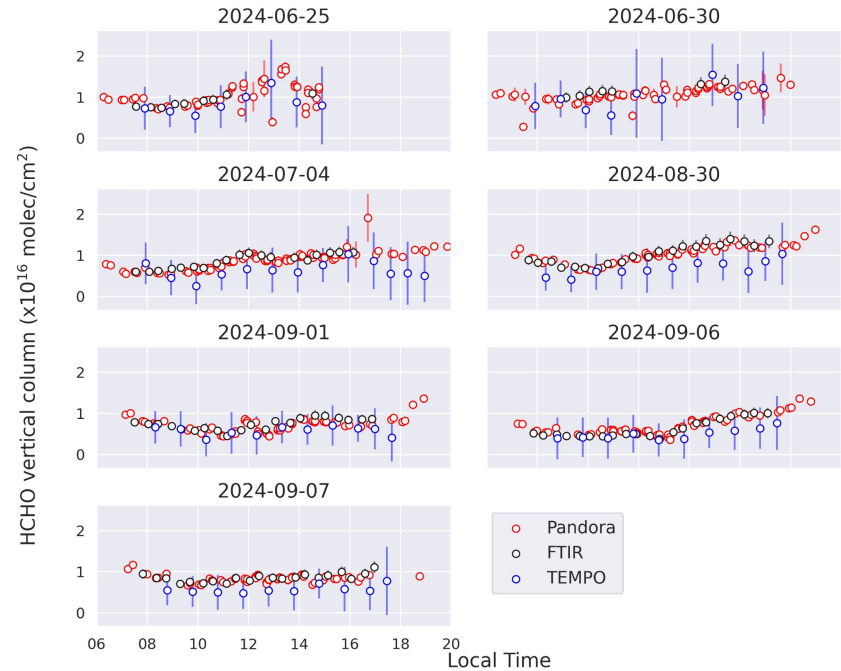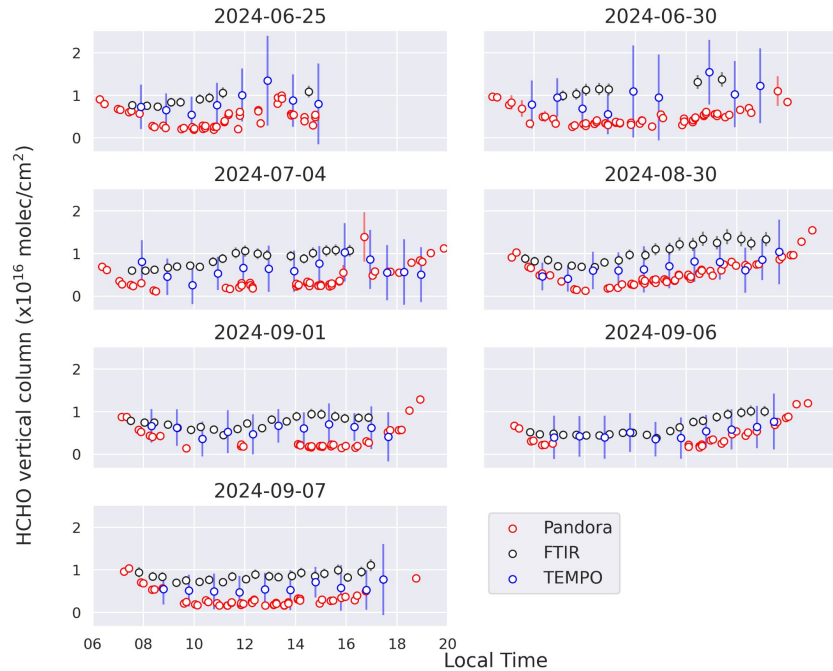*Before the correction*

After the correction
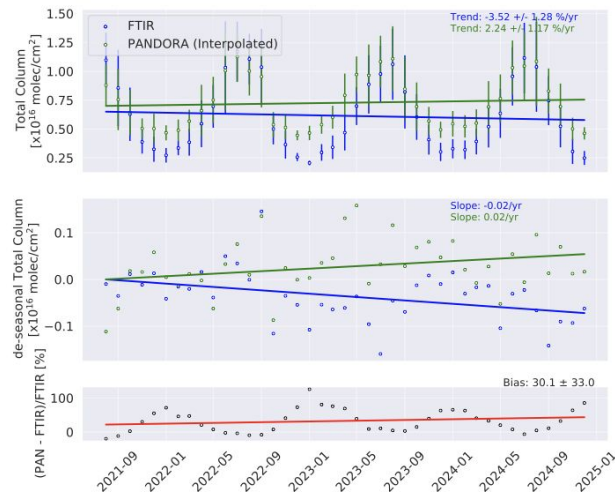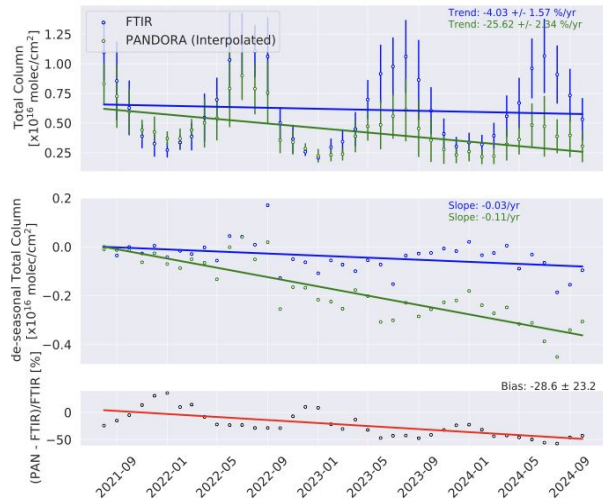
After correction trends are more similar. However, FTIR trends still compare better with Trop Columns (MAX-DOAS)
Now, pandora seems to be higher esp in the winter months.

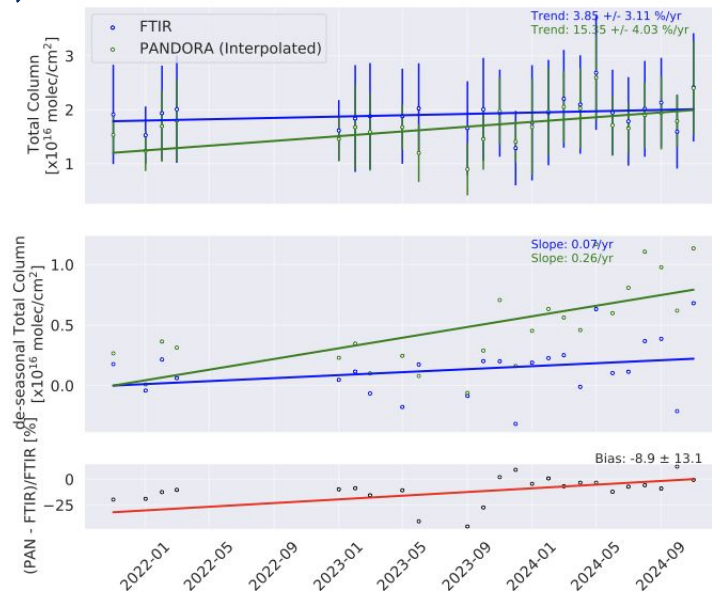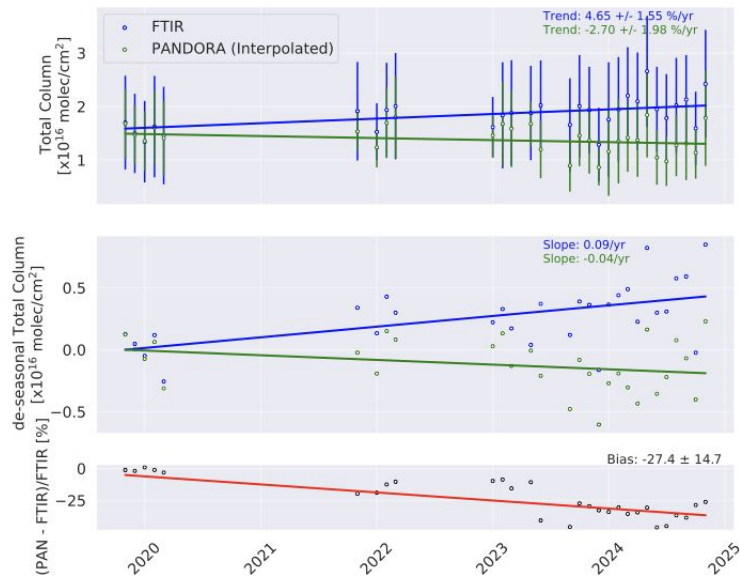# Example of diurnal comparison before and after correction

What about Mexico City and Toronto?

Mexico City
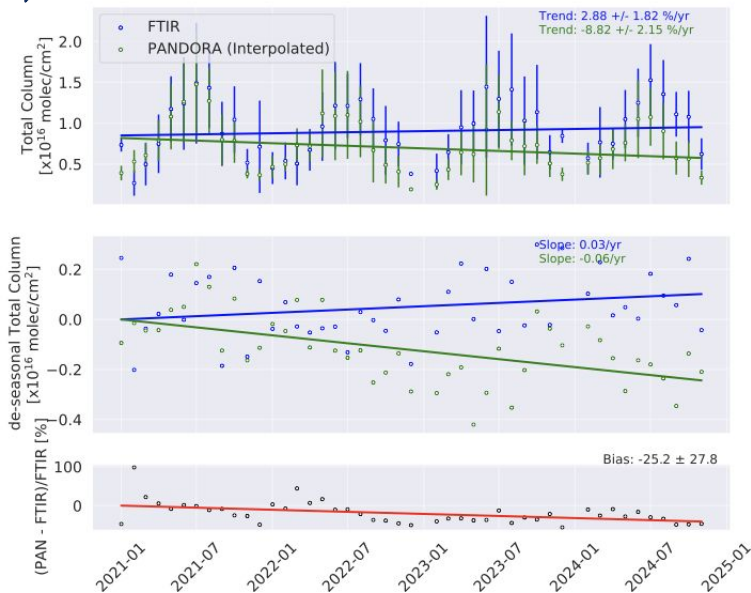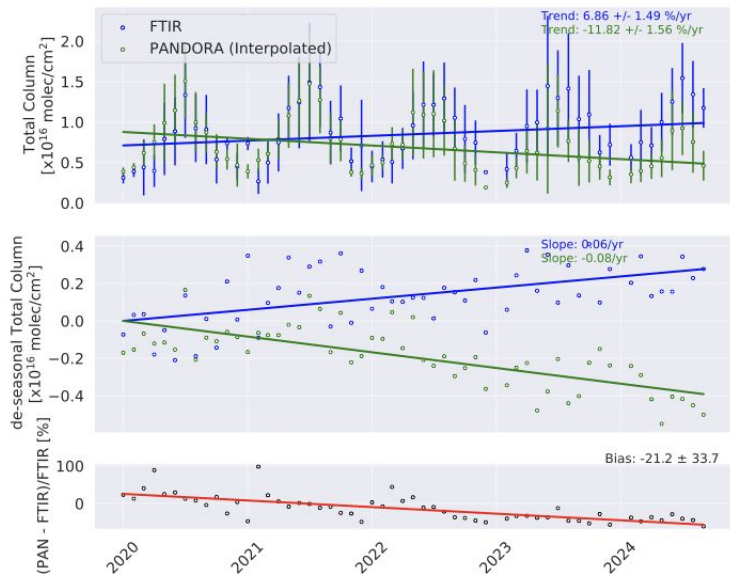
Before the correction → *After the correction*

After correction Pandora trend is now positive. However, FTIR trends still compare better with Trop Columns (MAX-DOAS). Bias between FTIR and Pandora improved.

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Before the correction → **After the correction**

After correction Pandora trend is less negative. However, FTIR trends still compare better with Trop Columns (MAX-DOAS). Bias between FTIR and Pandora remains the same.

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