Exploring biases in OCO full physics XCO_2 retrievals via realistic simulations of OCO-3 snapshot area maps

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1: Science Motivation

- Inferring carbon dioxide (CO_2) fluxes at urban-scales is a current topic of interest for both scientists and policy makers, e.g., (Ye et al., 2020, Wu et al., 2022, Wu et al. 2023, Che et al., 2024).
- Realistic simulations of Orbiting Carbon Observatory-3 (OCO-3) Snapshot Area Maps (SAMs) can be used to evaluate the ability to infer local and urban-scale fluxes from OCO-3 SAMs in the presence of realistic retrieval errors.
- High spatial resolution (2 km) WRF-Chem runs provide a unique set of realistic trace gases (including CO_2) and meteorology.
- Results are presented here for two cities (Phoenix, USA and Toronto, Canada).
- We demonstrate that in the simple "perfect knowledge" baseline case, XCO_2 can be retrieved with high fidelity, but oftentimes the combination of random instrument noise and aerosol effects confound the retrieval at levels that are likely to preclude accurate flux inferences.
- The primary goal of this effort is a prediction of realistic potential correlated errors on the scale of an OCO-3 SAM over urban areas.

2: OCO-3 Snapshot Area Mapping (SAM) mode

- OCO-3 has been making observations of column CO_2 (XCO_2) from the International Space Station since August 2019 (Taylor, et al., 2020).
- In addition to its nominal nadir and sun-glint viewing orientations, OCO-3 can target city-sized regions (80km by 80km) within approximately 2 minutes as it passes overhead via an agile 2D pointing mechanism. These observations are known as Snapshot Area Maps (SAMs) (Kiel, et al., 2021).
- Fig 1 indicates the location and type of SAMs acquired over the 4.25 year period from July 2019 through November 2023, at which time it was put into temporary storage, and is currently awaiting redeployment scheduled for July, 2024.
- The current work focuses on SAMs measured over the cities of Phoenix, USA and Toronto, Canada.

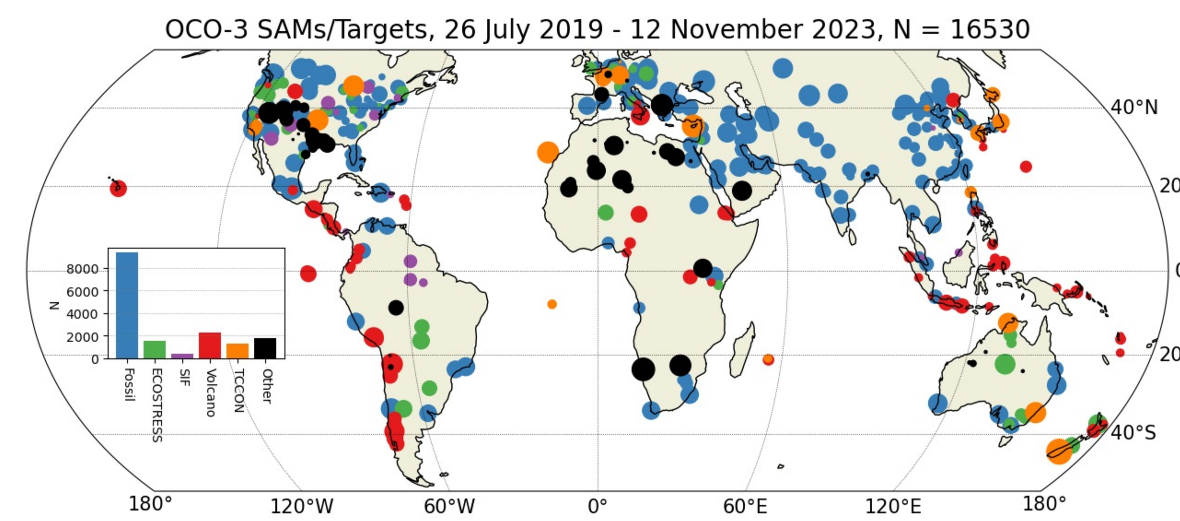

Fig. 1: Global map of location, type and density of OCO-3 SAMs.

3: The CSU Simulator and Retrieval Setup

- A codebase has been established that allows for the generation of realistic L1b radiance spectra from satellite instruments (McGarragh et al., 2024).
- In this work, scenes are generated using timing and geometry from actual OCO-3 SAMs.
- Meteorology and gases can be taken from a variety of sources, e.g, the NCEP, CAMS, GEOS-5, or WRF models.
- MODIS data are used for surface properties.
- In the current work, meteorology, trace gases, and aerosol fields are taken from realistic WRF-Chem model runs.
- Simulated spectra are cloud screened using the A-band Preprocessor (ABP) and flagged as either cloudy or clear.
- The clear soundings are run through the Atmospheric Carbon Observations from Space (ACOS) Level 2 Full Physics (L2FP) retrieval algorithm to produce estimates of XCO_2 with associated uncertainties.
- A simple linear bias correction against "dp" (retrieved – prior surface pressure) was applied to produce the final estimates of XCO_2.

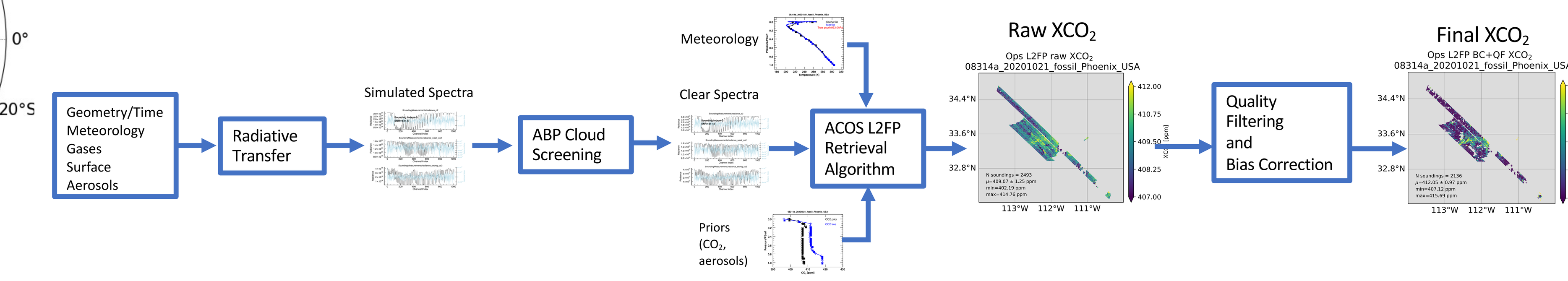

Fig. 2: Workflow of the CSU simulation system, including L1b spectra, cloud screening, L2FP retrieval, and quality filtering and bias correction to achieve final XCO_2 estimates.

4: Initial Results: Perfect Knowledge Baseline

- The perfect knowledge baseline setup has no aerosols included in either the simulated L1b spectra or the retrieval.
- In addition, there is a perfect match in spectroscopy and meteorology between the L1b and L2FP retrieval.
- Furthermore, the spectra do not include instrument noise.
- The surface model used was a simple Lambertian reflector for both L1b and L2FP, with L1b set to fixed albedo values per spectral band.
- In the perfect knowledge baseline case, the true WRF-Chem XCO_2 can be retrieved with mean bias $0.0 \pm <0.1$ ppm, and full range < 0.25 ppm.

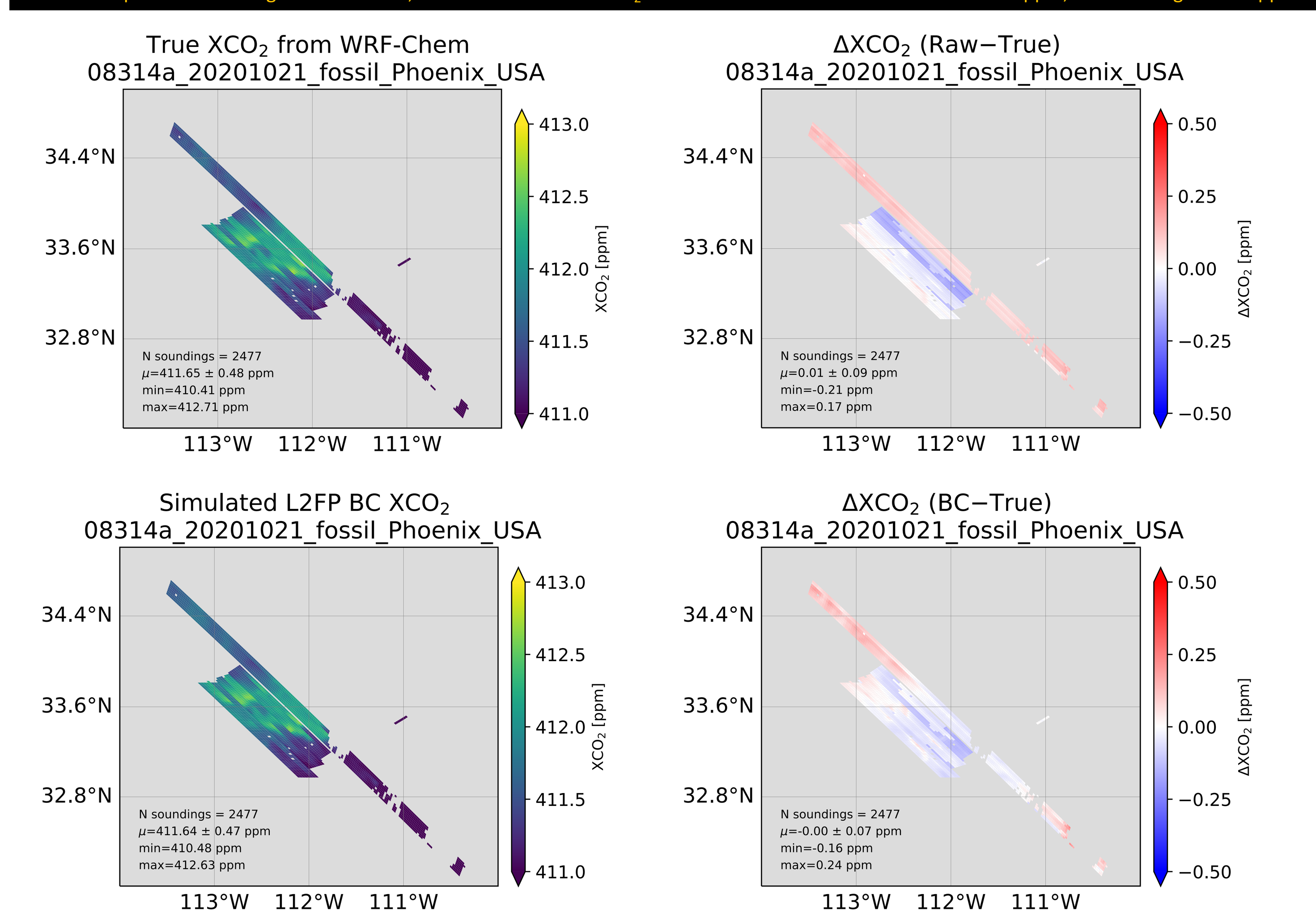

Fig. 3: True WRF-Chem XCO_2 (upper left), the final XCO_2 field after bias correction (upper right), scatter plot of the adjusted vs true XCO_2 field (lower left), and the bias corrected XCO_2 field (lower right) for the "perfect knowledge" setup.

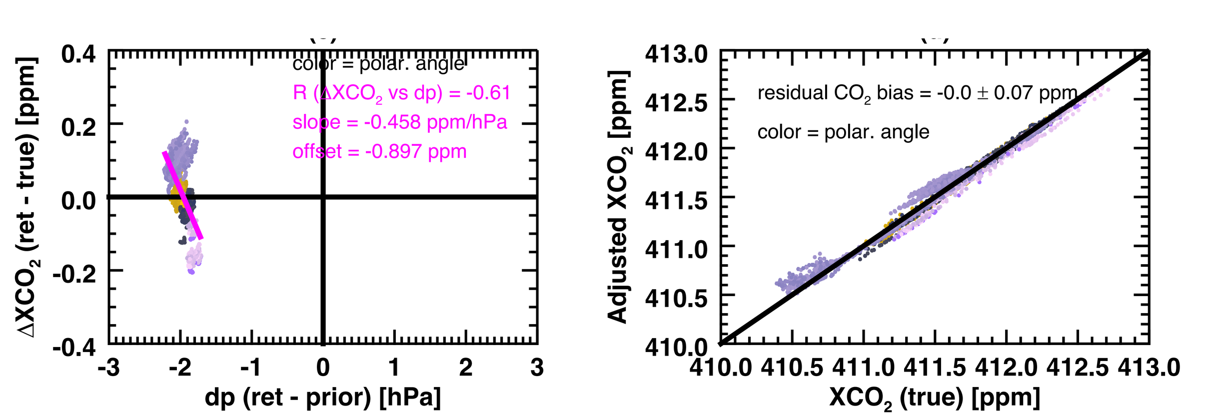

Fig. 4: Scatter plot showing the correlation of ΔXCO_2 with dp (left), and the corrected XCO_2 after bias correction vs the true value from WRF-Chem (right).

5: Initial Results: Simulations with Aerosols and Instrument Noise :: Case 1 (Phoenix 21-Oct-2020)

6: Initial Results: Simulations with Aerosols and Instrument Noise :: Case 2 (Toronto 08-Dec-2020)

- The introduction of mis-matched meteorology between L1b and L2FP, the additional of aerosols, and adding instrument noise to the L1b spectra, generally degrades the accuracy and precision of the XCO_2 estimates (Connor et al., 2016, McGarragh et al., 2024).
- These complications in the simulations generally lead to highly unphysical gradients in XCO_2 in the across-track direction, a phenomena termed "swath bias", in the OCO-3 SAMs (Bell et al., 2023).
- However, we find that the simple parametric bias correction against dp generally provides a correction to the XCO_2 estimates with mean bias of zero and scatter within the expected uncertainties of the retrievals (uncertainty < 0.5 ppm).

Case 1 (Phoenix)

- The initial retrieval of XCO_2 was biased 2.71 ± 1.04 ppm against the truth (upper row).
- After bias correction the XCO_2 field appears qualitatively similar to the true WRF-Chem field (lower left).
- The ΔXCO_2 field after bias correction appears as random scatter consistent with instrument noise with bias 0.00 ± 0.36 ppm (lower right).

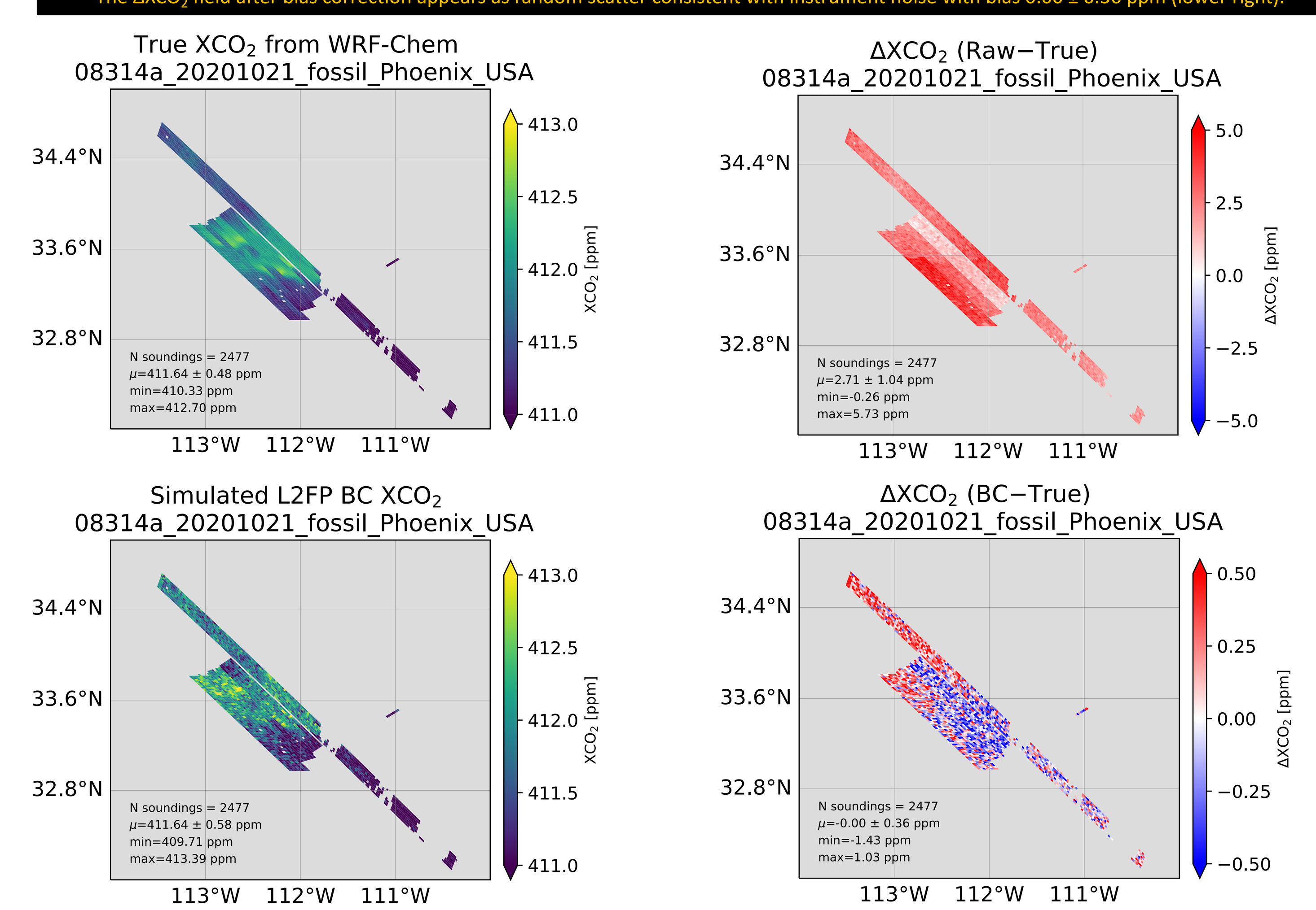

Fig. 5: True WRF-Chem XCO_2 (upper left), the initial difference versus the truth (ΔXCO_2) (upper right), the bias corrected XCO_2 field (lower left) and the final ΔXCO_2 (lower right).

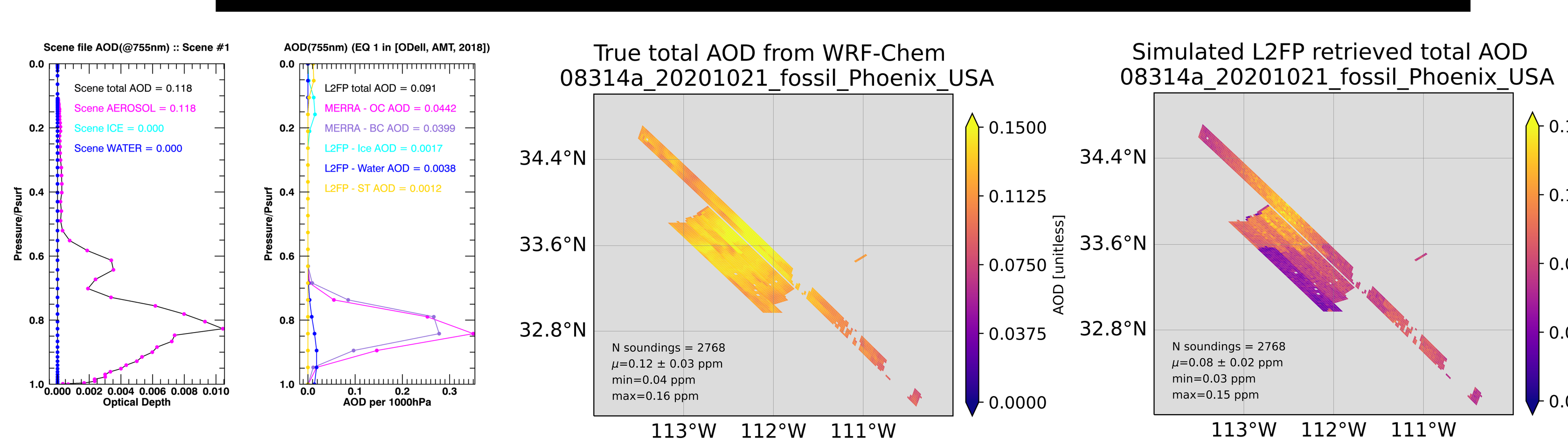

Fig. 6: Vertical profiles of aerosols for a select sounding in both the Scene file (left) and the L2FP output (center left). Map of the true AOD field from WRF-Chem (center right) and map of the L2FP retrieved AOD (right).

Case 2 (Toronto)

- The initial retrieval of XCO_2 was biased 1.13 ± 0.70 ppm against the truth (upper row).
- After bias correction the XCO_2 field appears qualitatively similar to the true WRF-Chem field (lower left).
- The ΔXCO_2 field after bias correction appears as random scatter consistent with instrument noise with bias -0.06 ± 0.43 ppm (lower right).

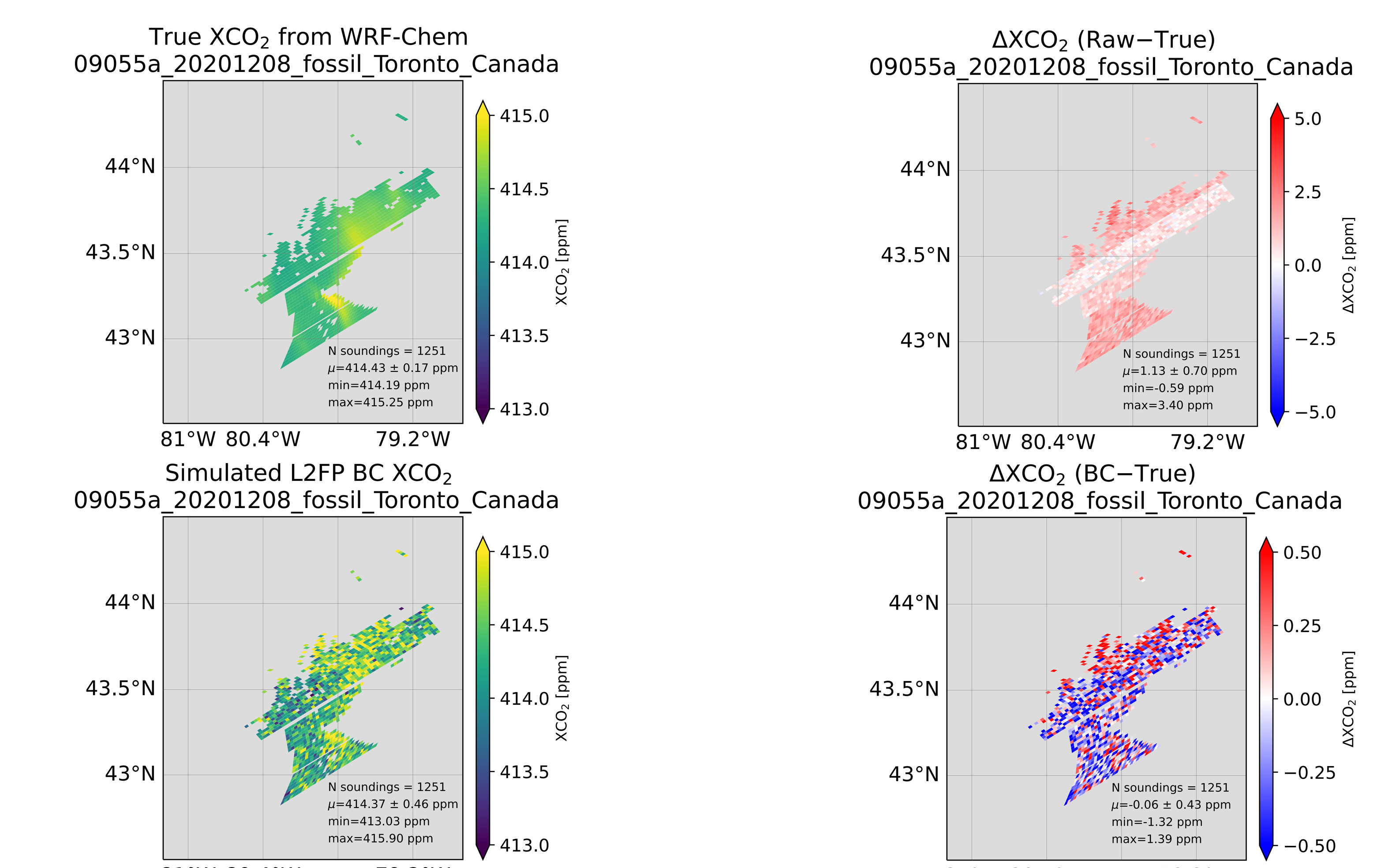

Fig. 7: True WRF-Chem XCO_2 (upper left), the initial difference versus the truth (ΔXCO_2) (upper right), the bias corrected XCO_2 field (lower left) and the final ΔXCO_2 (lower right).

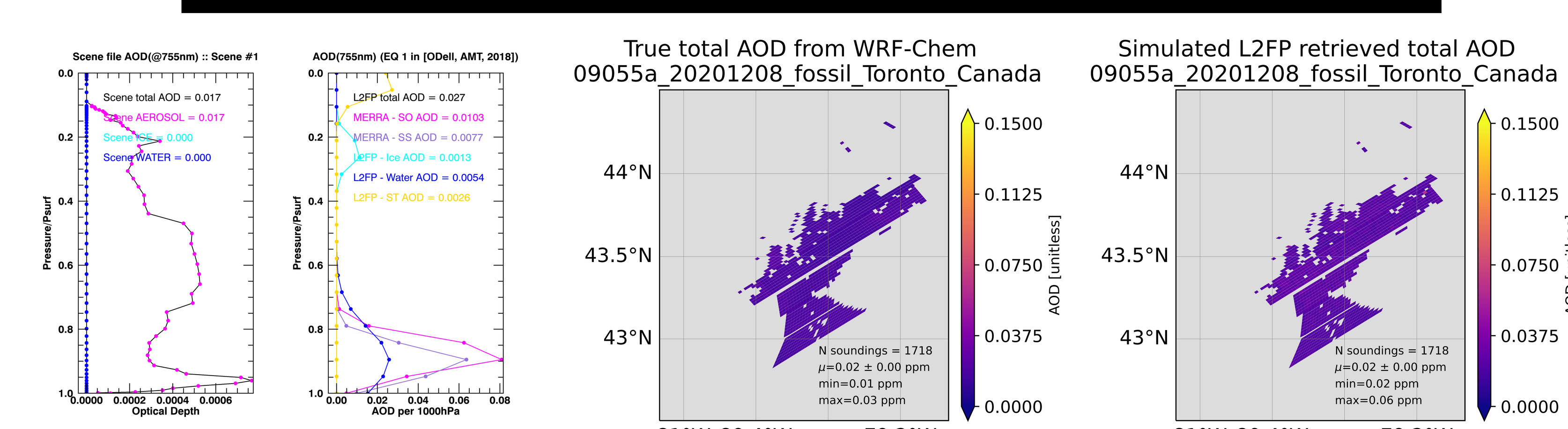

Fig. 8: Vertical profiles of aerosols for a select sounding in both the Scene file (left) and the L2FP output (center left). Map of the true AOD field from WRF-Chem (center right) and map of the L2FP retrieved AOD (right).

7: Summary and Initial Conclusions

- This work used geometry and timing from a set of OCO-3 Snapshot Area Mapping (SAM) mode observations, coupled with realistic meteorology, gases, and aerosols derived from high resolution WRF-Chem model runs to generate realistic spectra via radiative transfer calculations.
- After cloud screening, the clear spectra were run through the operational ACOS L2FP retrieval algorithm to produce raw estimates of XCO_2.
- A simple linear bias correction against "dp" (retrieved – prior surface pressure) was applied to produce the final estimates of XCO_2. No quality filtering is applied.
- When using the simple "perfect knowledge" setup, the final bias corrected estimates of XCO_2 are mean bias of 0.00 ± 0.07 ppm relative to the true values.
- With the introduction of instrument noise, mis-matched meteorology, and aerosol into the system, the estimates of XCO_2 generally contains swath biases and have large uncertainties of order 0.7 to 1 ppm versus the true values.
- However, the implementation of the linear bias correction largely mitigates the swath bias, leaving XCO_2 estimates with mean bias $0.0 \pm < 0.5$ ppm.

8: Next Steps and Future Work

- Additional sources of error still need to be explored, especially spectroscopy, which has been shown to be one of the largest known error sources in the retrievals after aerosols (Connor et al., 2016, McGarragh et al., 2024).
- Additional runs with more complex surface properties will be performed, as surface effects have also been shown to produce retrieval errors (Bell et al., 2023).
- The current work relies on a single parameter for bias correction (dp). A multi-parameter bias correction as is done for operational OCO data using , e.g., aerosol and albedo fields, will likely improve the results (O'Dell et al., 2018).
- WRF-Chem runs have been performed for two additional days for three cities (including Cairo, Egypt which was not shown here).
- We will continue to explore the results and look for explanatory variables that might help deduce issues within the L2FP retrieval for possible improvement to provide better estimates of XCO_2.

9: References

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