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Tropospheric Formaldehyde Retrievals from GEMS within the GEO-RING Project

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01 Introduction

Formaldehyde (HCHO) is a short-lived product of volatile organic compound oxidation and a key precursor of tropospheric ozone, making it an essential proxy for surface emissions and air quality.

Until recently, global HCHO monitoring relied on low-Earth-orbit (LEO) sensors, providing limited temporal coverage. The advent of geostationary UV–visible spectrometers such as GEMS, TEMPO, and Sentinel-4 now enables continuous daytime observations over Asia, North America and Europe.

Within the Geo-Ring project, we evaluate the GEMS operational HCHO product and explore methods to improve the retrievals. To enhance the DOAS inversion, we test two approaches: (1) pseudo-cross-sections derived from principal component analysis of fit residuals, and (2) a CODOAS approach exploiting the covariance of the fit residuals. These methods are designed to be applicable consistently across GEMS, TEMPO, and Sentinel-4 to mitigate instrumental artifacts and scene inhomogeneity.

We also revisit background correction and air mass factor calculations for GEO observations, ensuring compatibility with LEO-based HCHO climate data records (ESA CCI).

Finally, GEMS data are analysed to characterise diurnal variability over selected regions.

04 Background correction

$$VCD = (SCD - SCD_0) / AMF + VCD_0$$

Final VCDs combine destriping and SCD negative offset (SCD_0), and a model-based background term (VCD_0):

- Per-row fit of HCHO SCD vs. O_3 SCD → SCD_0
- Pixel filtering: max RMS, max SCD, max SZA/VZA, max CF
- VCD_0 from CAMS free-troposphere model + spatial smoothing, emissions excluded.

Final VCDs are sensitive to background-correction settings (source of uncertainty).

Persisting band structures over the Indian Ocean (see also Fig.5).

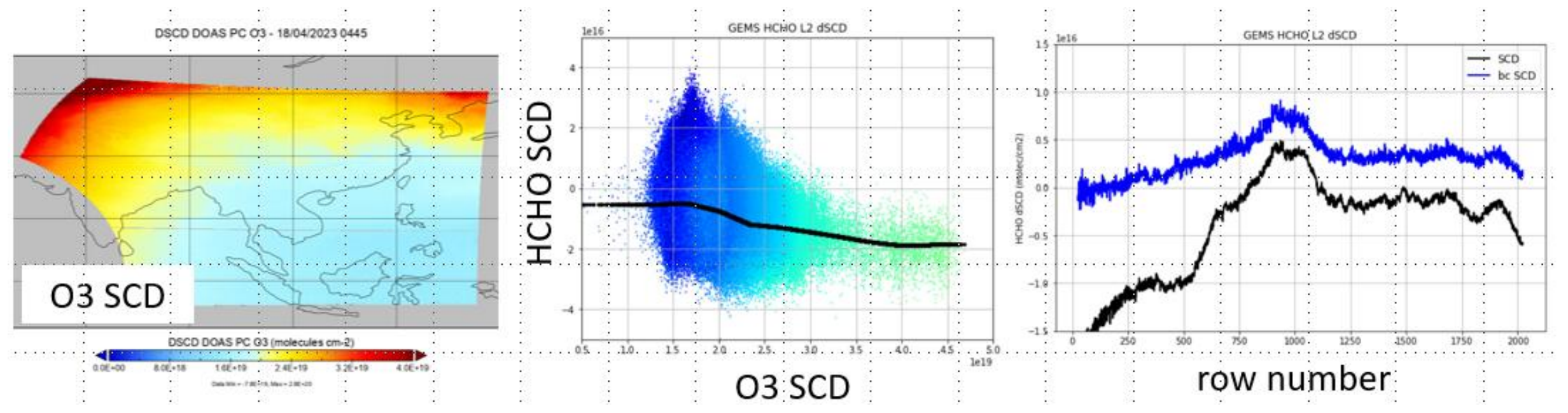

Fig. 4 : Background correction based on the O3 SCD for each row.

02 CODOAS Method

We use a Covariance-DOAS (CODOAS, Theys et al., 2025) approach exploiting the covariance of fit residuals to improve HCHO SCD precision over heterogeneous scenes (no reference sector required).

1. Perform a classical DOAS fit → HCHO SCDs.
2. Spatially smooth the HCHO SCDs → HCHO optical depths.
3. Subtract HCHO optical depths from radiances.
4. Perform a second DOAS fit (without HCHO) → wavelength-dependent residuals.
5. Compute the covariance matrix of the residuals (or the PCA eigenvectors).
6. Perform a third DOAS fit on the original radiances using the covariance matrix as weighting (or the PCA terms as pseudo cross-sections).

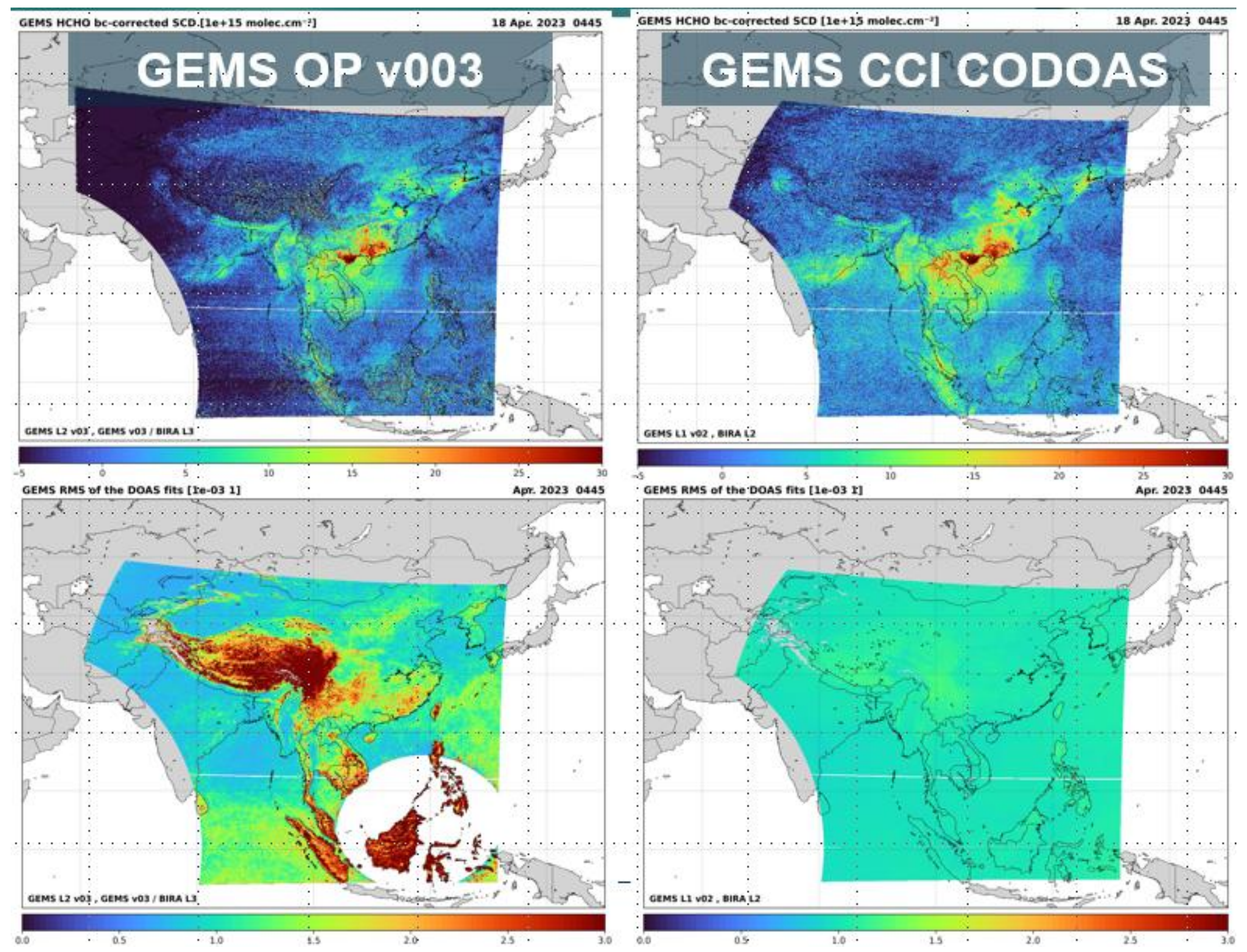

Fig. 1: HCHO SCD and RMS in the operational product and with CODOAS for one GEMS scene.

DOAS settings

Fitting interval	**328.5-359 nm**
Cross-sections	HCHO 298K (Meller and Moortgat, 2000), O_3 223K and 243K (Serdyuchenko et al., 2014) with solar Io correction + non-linear absorption terms (Pukite et al., 2010), BrO 223K (Fleischmann et al., 2004), NO_2 294K (Vandaele et al., 1998), O_2-O_2 293K (Thalman and Volkamer, 2013), Ring (Chance and Spurr, 1997), GEMS polarization sensitivity spectrum.
Polynomial	5th order
Intensity offset	Linear, 1st order
Wavelength shift/stretch	Linear approach, Beirle et al., 2013
Reference spectrum	**Daily irradiance**

03 Air Mass Factors

AMFs are computed using CCI settings, ensuring compatibility with the HCHO ESA climate data record (LEO CDR):

- TROPOMI surface albedo (min LER at 340 nm)
- CAMS Rea a priori profiles (3-hour resolution)
- Baseline: clear-sky AMF + cloud filtering
- Cloud fractions are taken from the IUP Bremen GEMS NO_2 product

➢ Clear-sky AMFs are similar between GEMS and TROPOMI CCI products.
➢ CCI AMFs are generally lower than the GEMS operational AMFs.

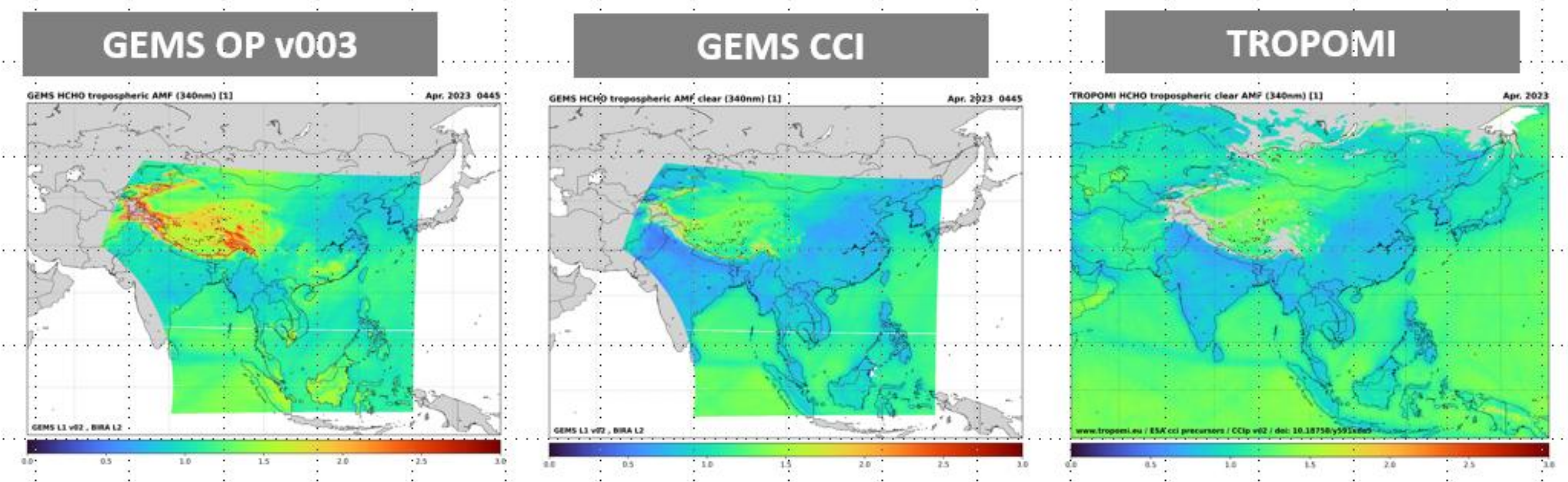

Fig. 3 : Comparison of AMF GEMS operational vs CCI settings.

05 Results

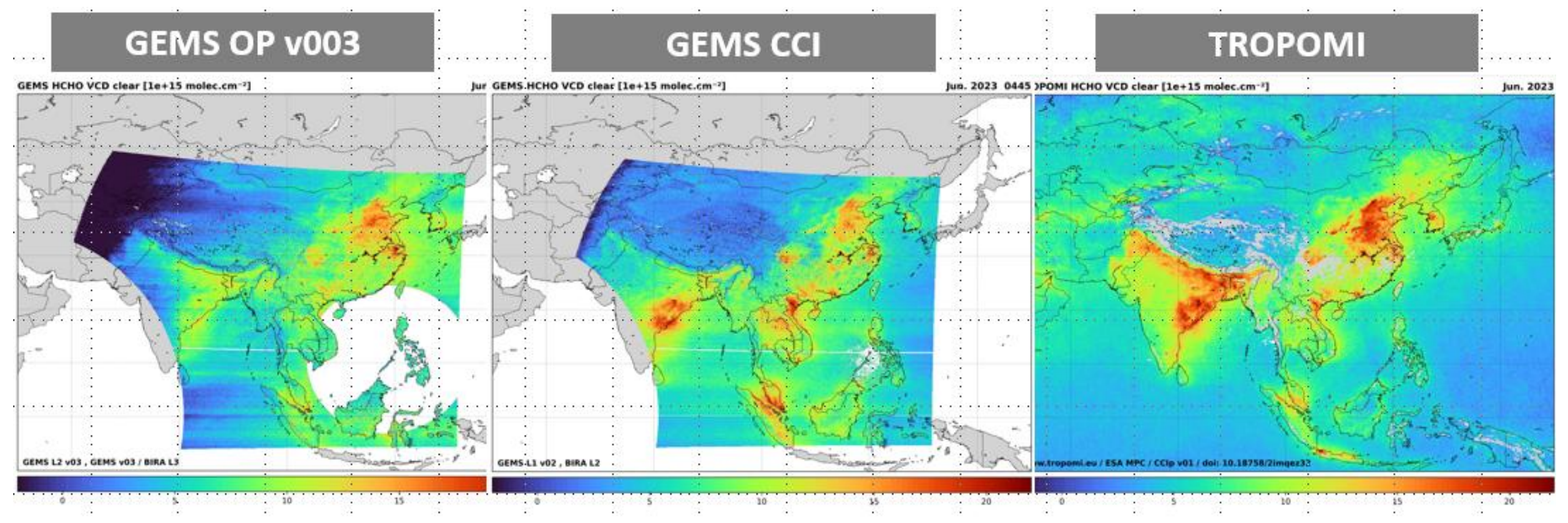

Fig. 5 : Mean tropospheric HCHO VCD (June 2023): GEMS operational v003, CCIp, TROPOMI reference.

Information content

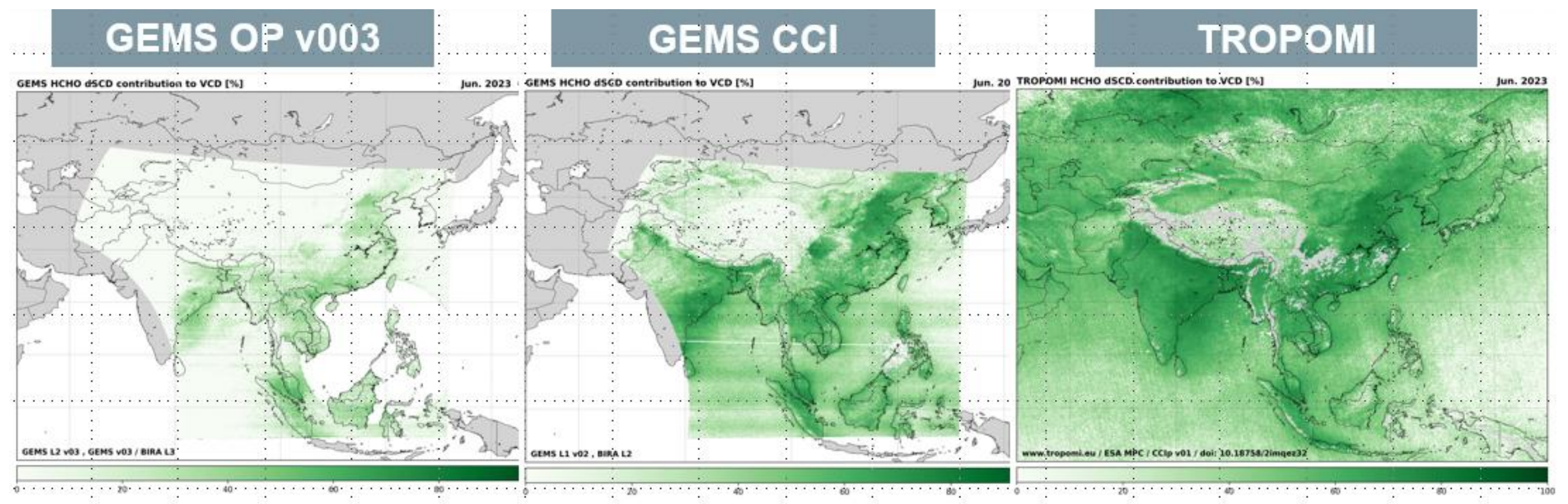

Fig. 5b: Tropospheric HCHO information content, fraction of VCD originating from the measurement (vs. model background): GEMS OP v003, GEMS CCIp, TROPOMI.

06 Regional Time Series

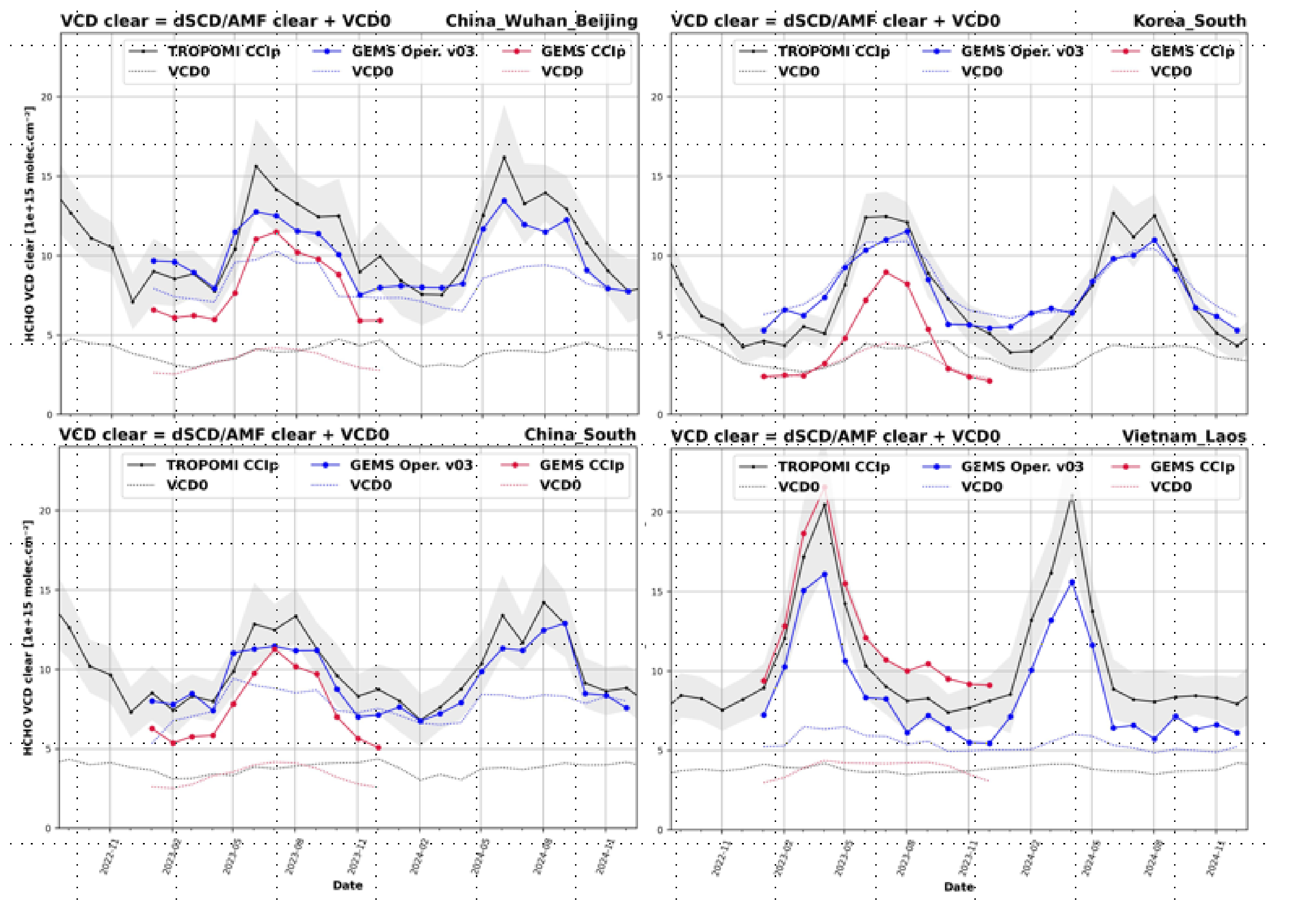

Fig. 6 : Time series of monthly mean HCHO VCD (and VCD_0 contribution) over 4 regions: Beijing area, South Korea, Southeastern China and Vietnam/Laos.

- Excessive model contribution to HCHO VCDs in GEMS operational v003.
- GEMS CCIp HCHO VCD show a negative bias in NE Asia, but with a larger information content (smaller VCD_0 contribution).

07 Diurnal Variations

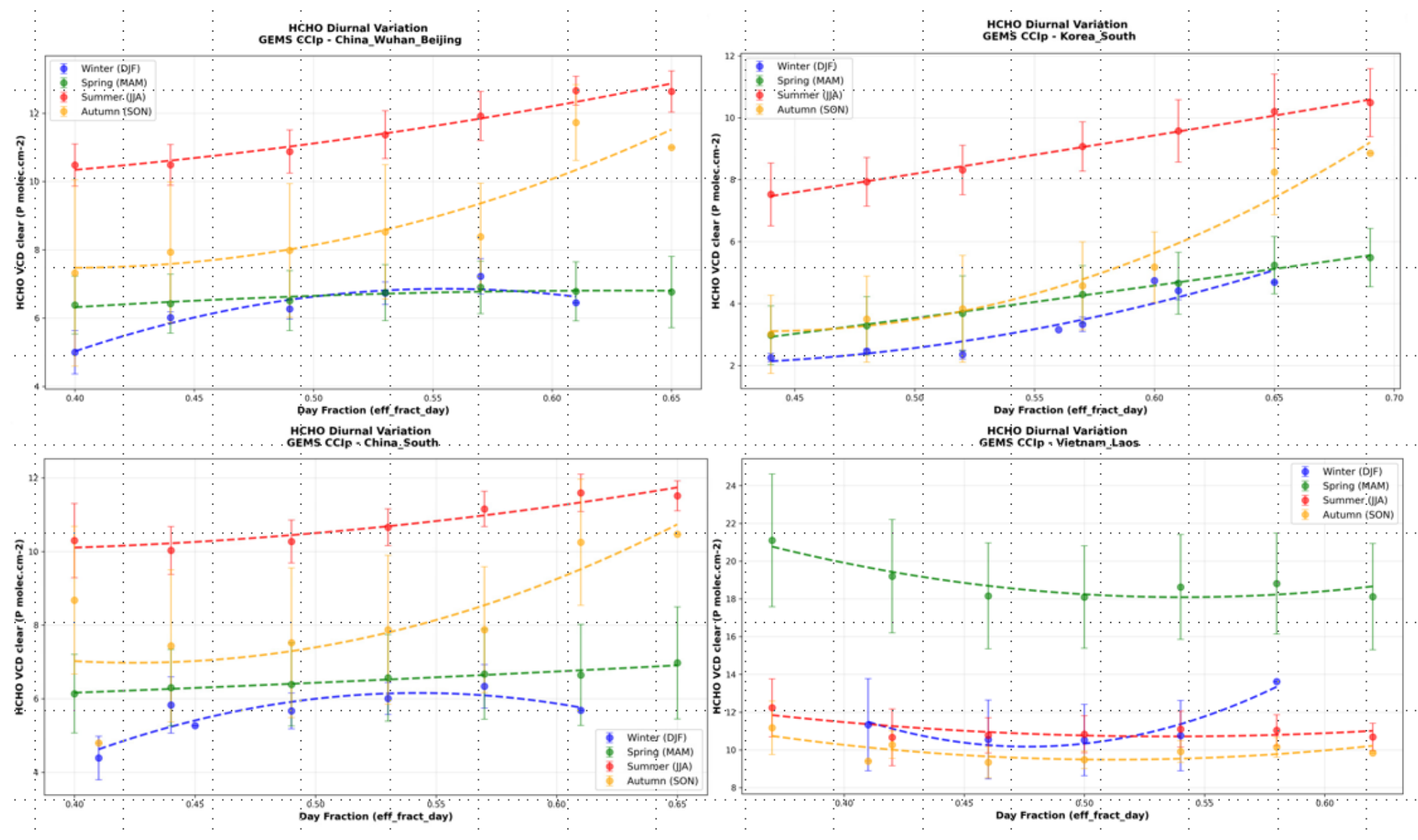

Fig. 7 : Seasonal diurnal cycles derived from the CCIp product over the 4 regions of Fig.6.

- Spring–summer urban regions: clear daytime increase of HCHO columns, consistent with enhanced photochemical production from VOC emissions.
- Spring biomass-burning regions: higher HCHO columns in the morning, possibly reflecting limited early-day photochemical loss.

- A complete L3 dataset for GEMS HCHO in 2023 has been produced within GeoRing and CCIp.
- CODOAS allows for a reduction of fitting RMS and SCD noise over heterogeneous scenes.
- Using consistent auxiliary data brings the GEMS AMFs closer to the TROPOMI AMFS, and generally lower than in the operational product.
- Differences in AMF can explain 25% of the differences between the GEMS and TROPOMI operational products in summer.
- The refined background correction allows for enhanced information content, with much reduced model-emission contribution.
- A persistent negative bias is overserved over Northeastern Asia and Northern India.

Outlook

- Sensitivity to BC settings under investigation.
- Assess performance against ground-based networks (PGN Pandora, NDACC FTIR and MAX-DOAS).
- Compare the diurnal variation with combined morning and afternoon LEO observations.
- Apply CODOAS and background correction scheme to S4 and TEMPO.
- Investigate the impact of the GEMS irradiance on the SCD bias.

References: *De Smedt et al. (2025); Theys, CODOAS, DOAS Workshop 2025; Richter et al. (GEMS NO_2 IUPB product); ESA CCI+ Precursors.*
De Smedt, I., Vlietinck, J., Yu, H., Theys, N., Danckaert, T., & Van Roozendael, M. (2025). CCI+P HCHO tropospheric column L3 data from TROPOMI, v2 (Version 2) [Data set]. https://doi.org/10.18758/y591kda5

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