2022.11.09. The 13th GEMS international workshop

Current status of GEMS VOCs and their scientific applications

Rokjin J. Park[1)], Gitaek Lee[1)], Eunjo S. Ha[1)] Sieun D. Lee[1)], Hyeong-Ahn Kwon[2)], Christophe Lerot[3)], Corinne Vigouroux[3)], Francois Hendrick[3)], Isabelle De Smedt[3)], Michel Van Roozendael[3)], and Pucai Wang[4)]

[1)]School of Earth and Environmental Sciences, Seoul National University, Korea

[2)]Department of Environmental & Energy Engineering, University of Suwon, Korea

[3)]Belgian Institute for Space Aeronomy, Brussels, Belgium

[4)]Chinese Academy of Sciences, Beijing, China

Atmospheric Chemistry Modeling Group, Seoul National University

Updates of GEMS HCHO retrieval algorithm (v1.2.0)

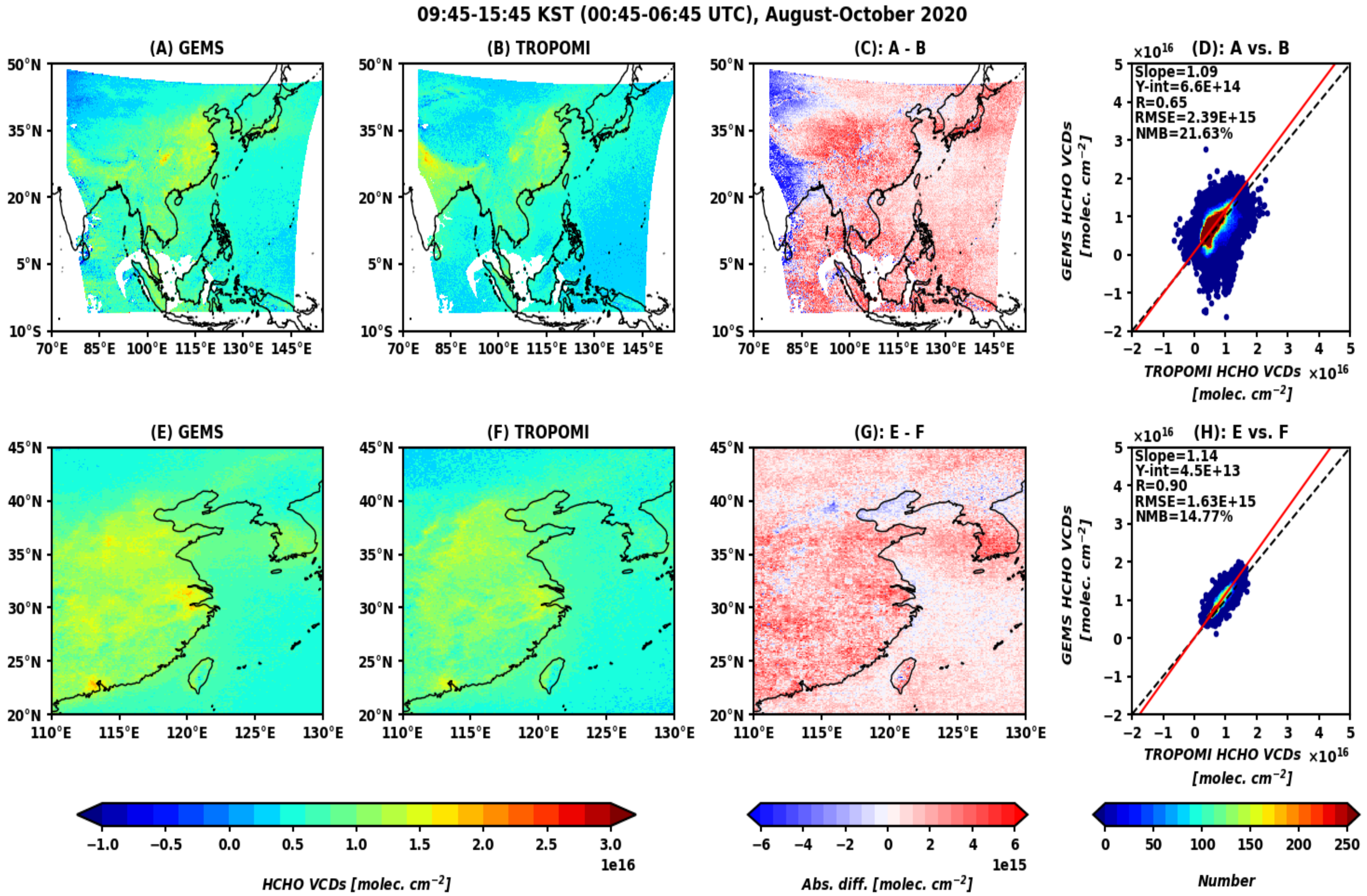
[Major updates of GEMS HCHO v1.2.0]

- **Polarization correction**
  - Polarization sensitivity vectors are included as a pseudo-absorber in the spectral fitting.
- **Updated absorption cross-sections**
  - O_3 (Serdyuchenko *et al*., 2014)
  - O_4 (Finekenzeller and Volkamer, 2022)
- **Updated Fitting window**
  - 328.5-356.5 nm → 329.3-358.6 nm
- **The use of three days mean radiance references**
  - Mean radiance references from the previous two days' observations are used.
  - Sufficiently fill missing latitudinal points of the reference spectra.
- **A priori profile**
  - WRF-Chem + CAM-Chem 28 x 28 km → GEOS-Chem 0.5 x 0.625 deg.
  - Considers recent emission inventories and meteorological fields.

Fitting window (calibration window)	329.3-358.6 nm (326.3-361.0 nm)
Fitting method	Direct fitting [González Abad *et al.*, 2015]
Absorption cross-sections	HCHO, O_3, NO_2, BrO, O_4, Ring effect, polarization sensitivity
Polynomials	Third order
Reference spectrum	120°E ~ 150°E zonal mean radiances [Filtering option] ✓ cloud fraction < 0.4

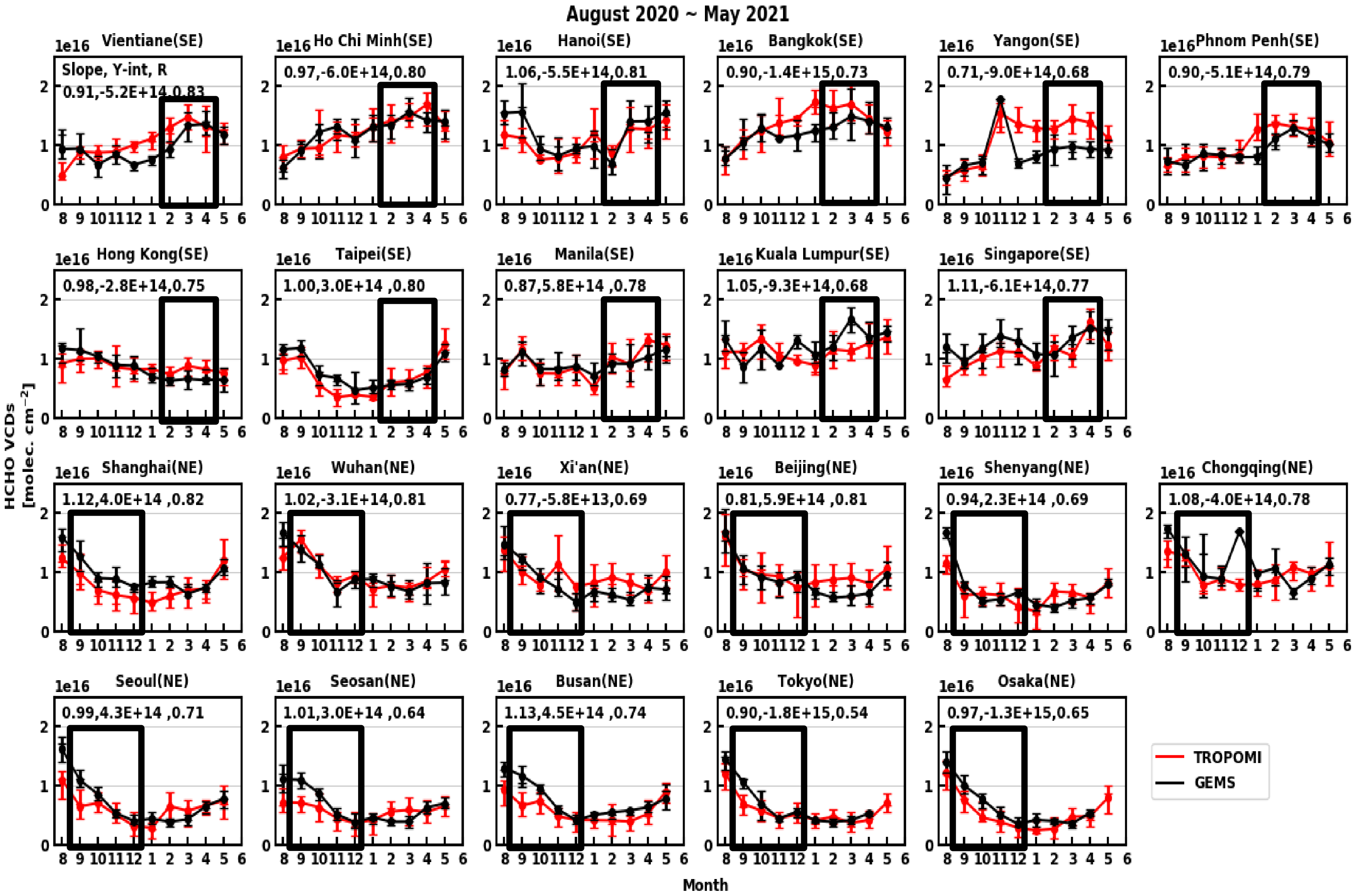
Poster by Gitaek Lee
Evaluation of GEMS HCHO vertical column densities

HCHO VCDs comparison: GEMS vs. TROPOMI

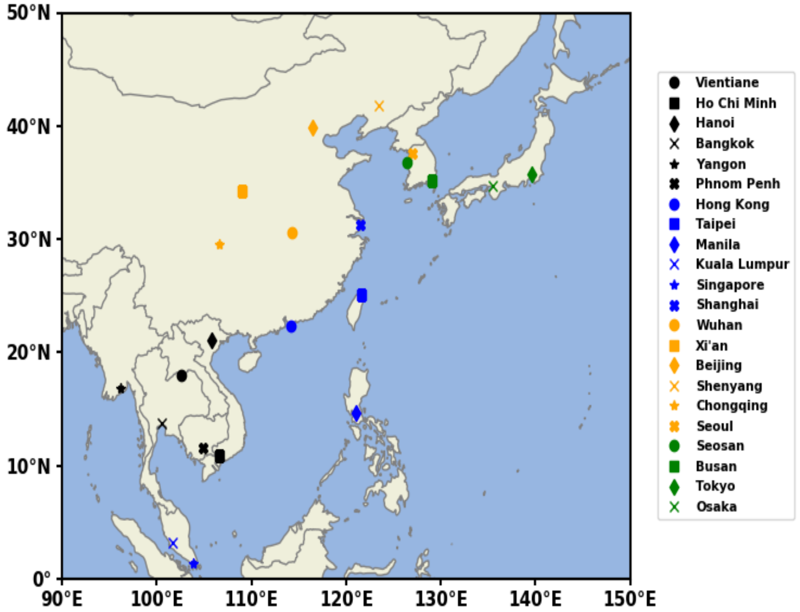


Seasonal variation of HCHO VCDs: GEMS vs. TROPOMI

* Preliminary results



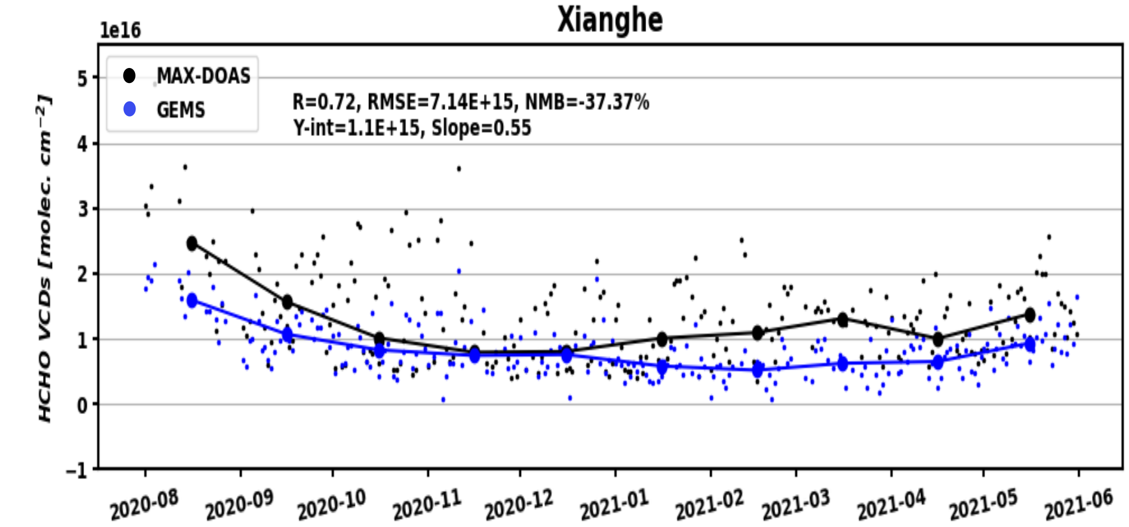
2020.08. ~ 2021.05.
TROPOMI overpass time



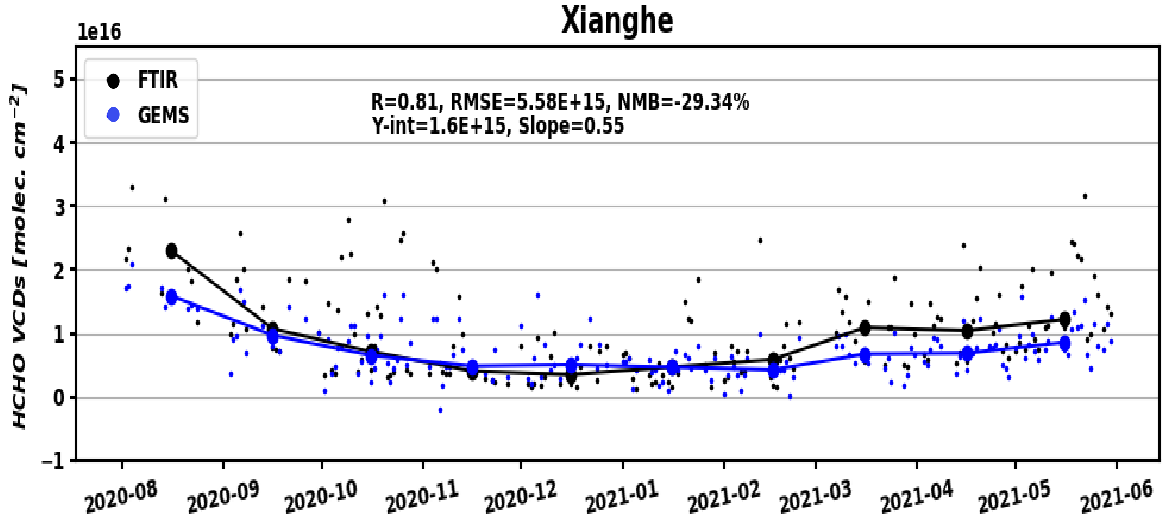
SE: Southeast Asia
NE: Northeast Asia

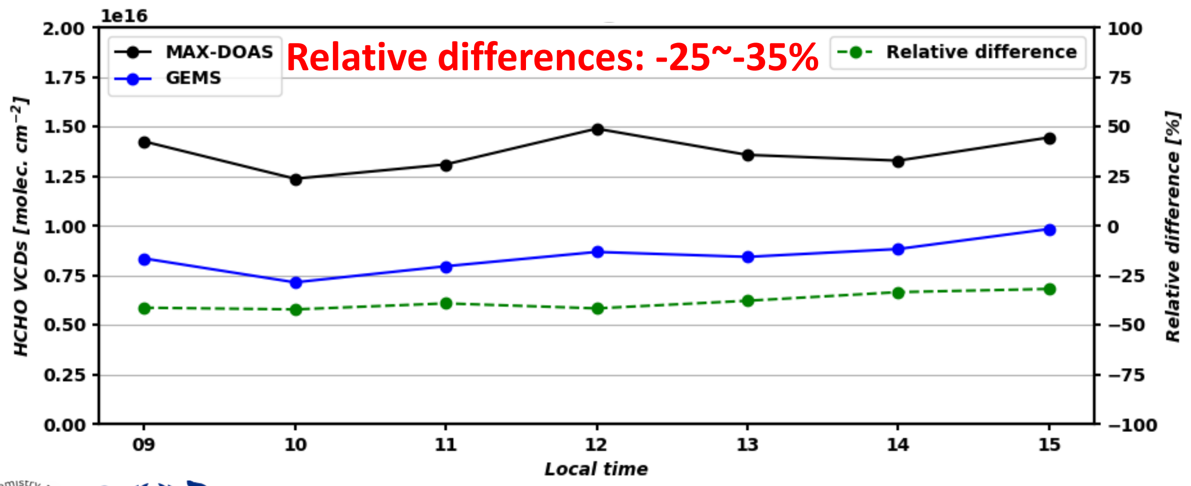
HCHO VCDs comparison:
GEMS vs. ground-based observations (MAX-DOAS, FTIR)

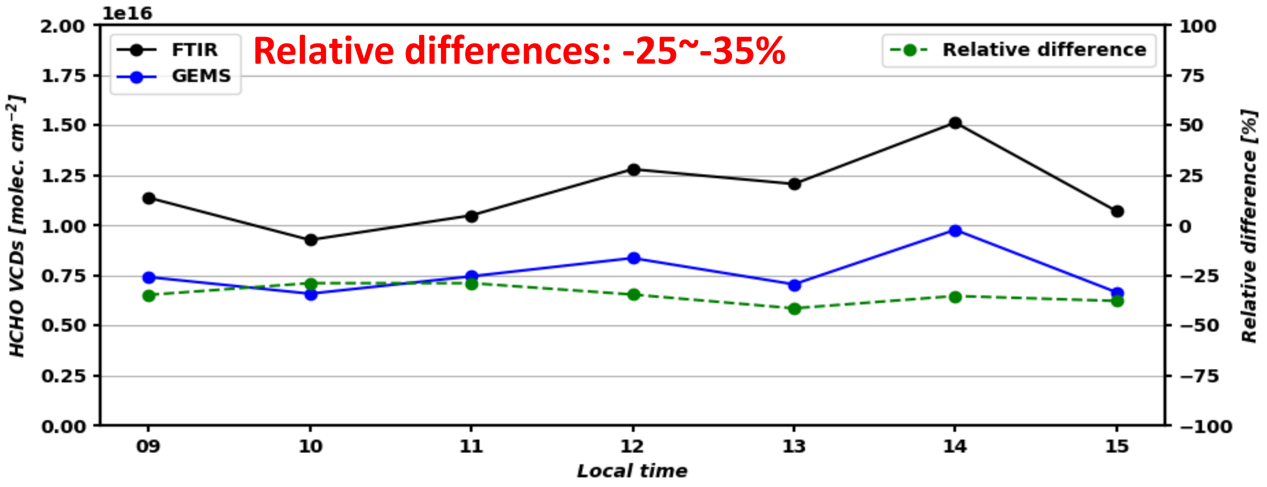
GEMS vs. MAX-DOAS



GEMS vs. FTIR

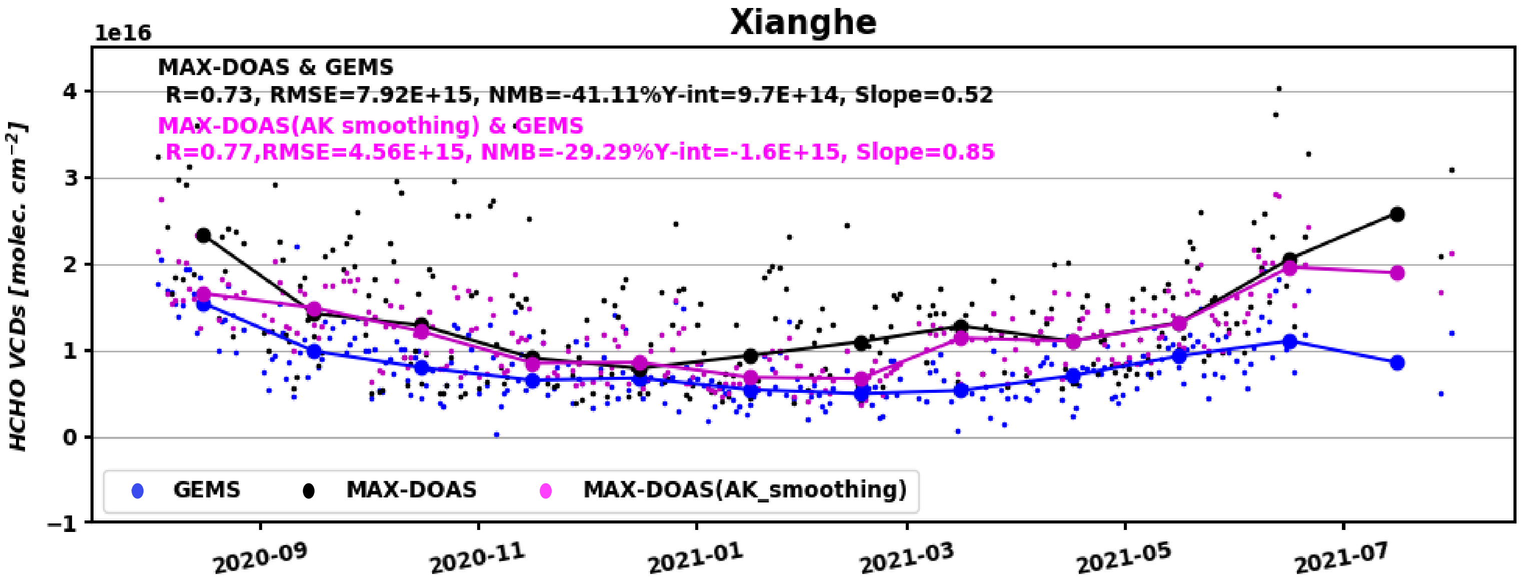


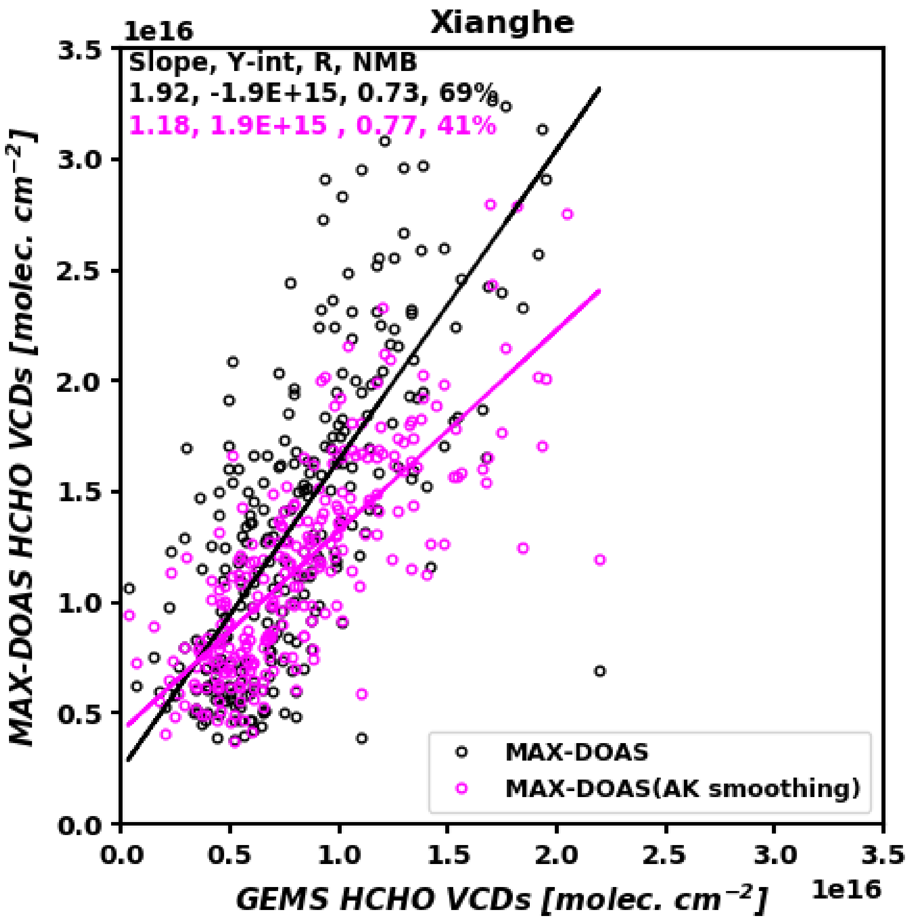




Small marker: daily mean
Large marker: monthly mean

HCHO VCDs comparison:
GEMS vs. MAX-DOAS applied with GEMS AK





Small marker: daily mean
Large marker: monthly mean

Updates of GEMS CHOCHO retrieval algorithm (v1.2.0)

[Major updates of GEMS CHOCHO v1.2.0]

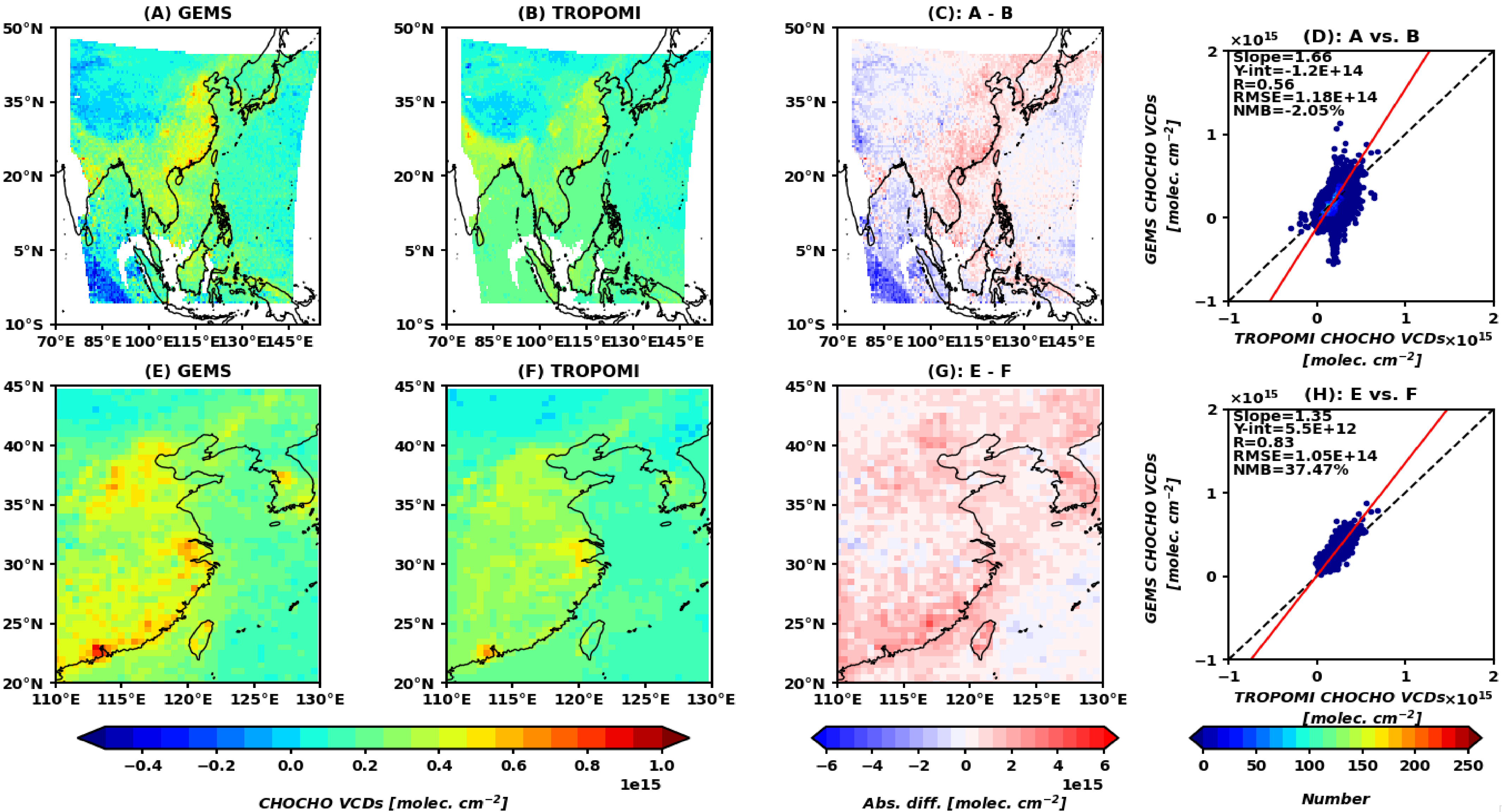
- **Polarization correction**
  - Polarization sensitivity vectors are included as a pseudo-absorber in the spectral fitting.
- **Updated absorption cross-sections**
  - O_3 : Serdyuchenko *et al.*, 2014
  - O_4 : Finkenzeller and Volkamer, 2022
  - H_2O (vapor) : HITRAN 2020
  - H_2O (liquid) : Mason et al., 2016
- **Updated Fitting window**
  - 433-458 nm → 433-461.5 nm
- **The use of three days mean radiance references**
  - Mean radiance references from the previous two days' observations are used.
  - Sufficiently fill missing latitudinal points of the reference spectra.
- **A priori profile**
  - Monthly mean GEOS-Chem 2 x 2.5 deg. → Monthly mean hourly GEOS-Chem 0.25 x 0.3125 deg.

Fitting window (calibration window)	433-461.5 nm (431-463.5 nm)
Fitting method	Direct fitting [González Abad *et al.*, 2015]
Absorption cross-sections	CHOCHO, O_3, NO_2, O_4, H_2O (vapor), H_2O (liquid), Ring effect, polarization sensitivity
Polynomials	Third order
Reference spectrum	120°E ~ 150°E zonal mean radiances [Filtering option] ✓ cloud fraction < 0.4

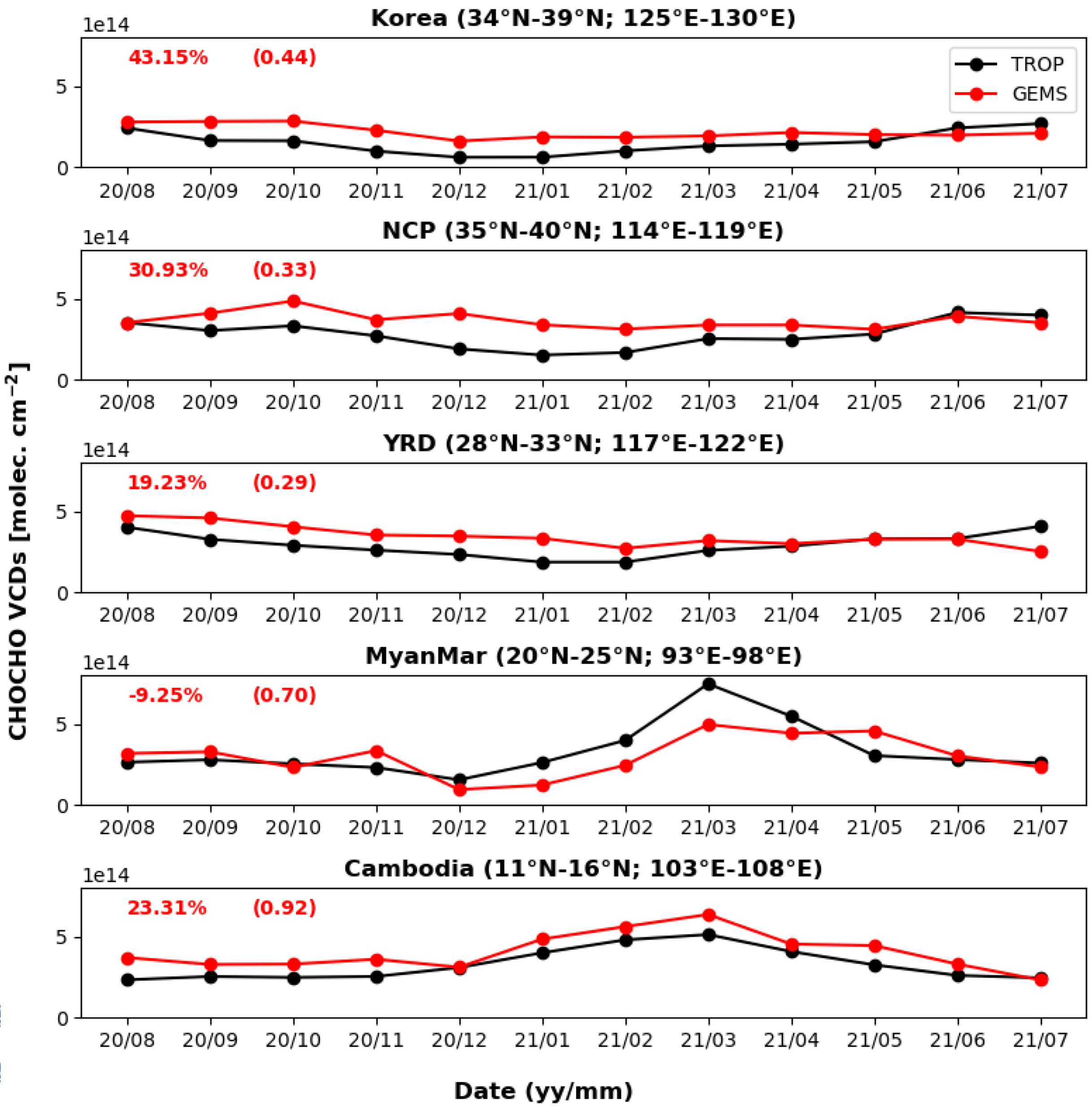
Poster by Eunjo Ha
Evaluation of GEMS glyoxal vertical column densities

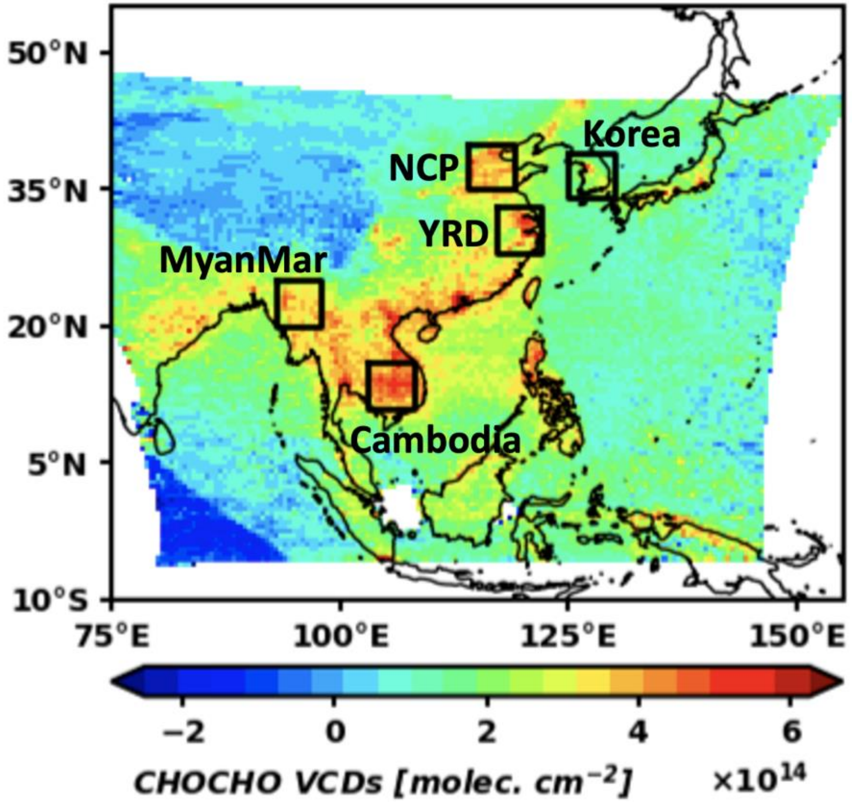
CHOCHO VCDs comparison: GEMS vs. TROPOMI

09:45-15:45 KST (00:45-06:45 UTC), August-October 2020



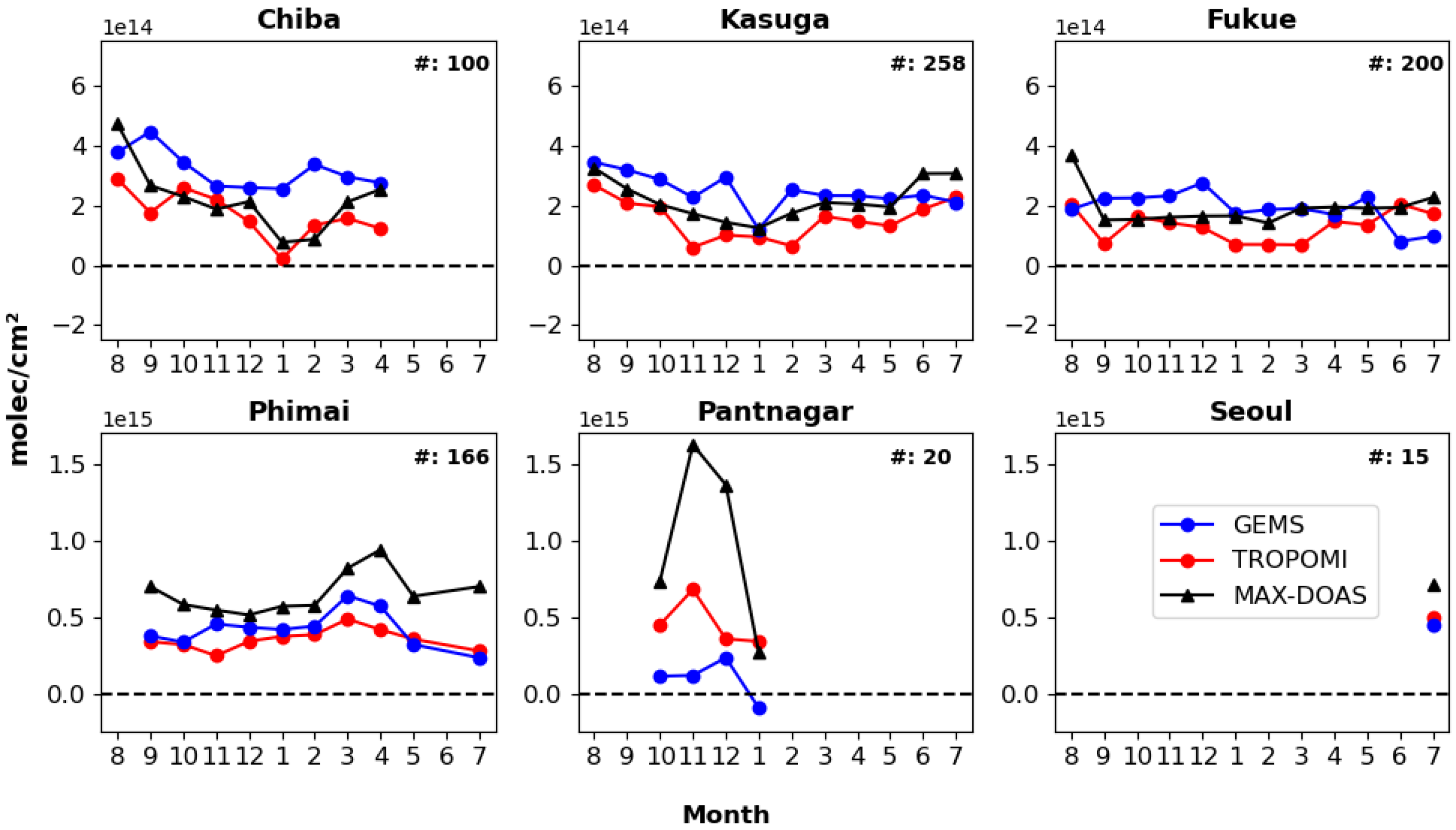
Seasonal variation of CHOCHO VCDs: GEMS vs. TROPOMI





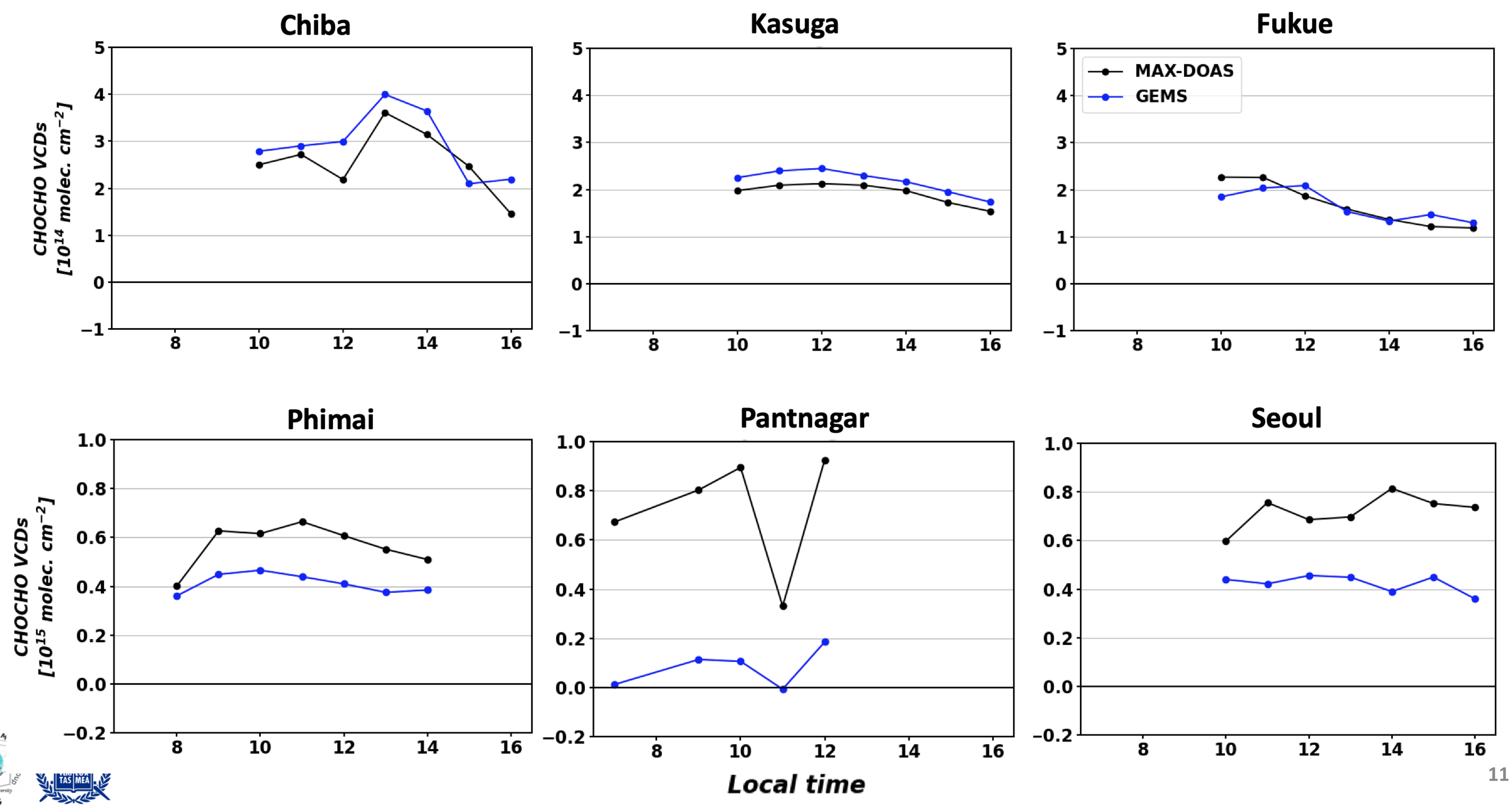
* NCP : North China Plain, YRD : Yangtze River Delta

Seasonal variation of CHOCHO: GEMS vs. MAX-DOAS



#: Number of hourly averaged data

Diurnal variation of CHOCHO VCDs: GEMS vs. MAX-DOAS



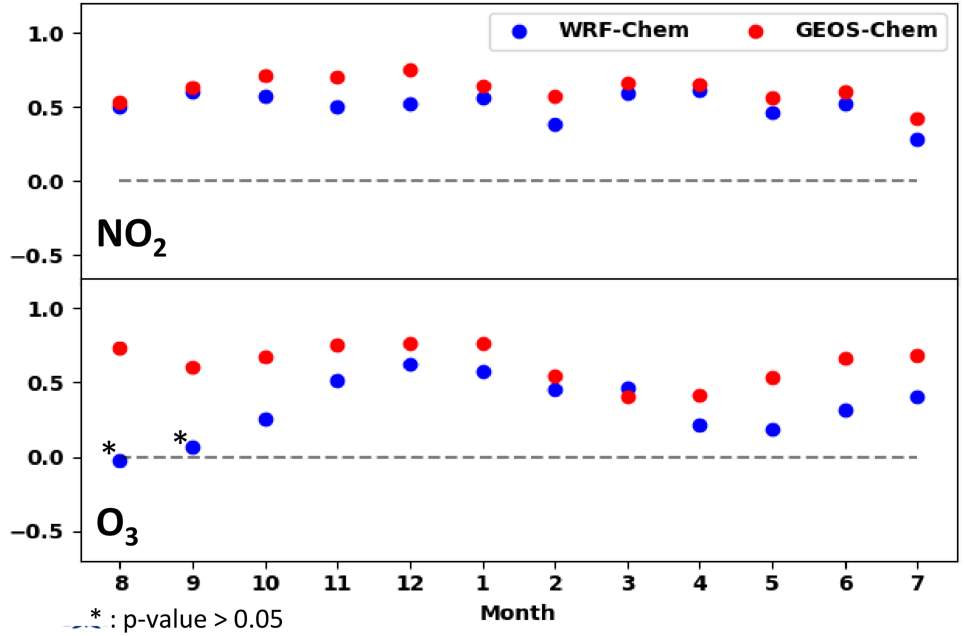
Change in a priori profile data

Poster by Sieun Lee
Sensitivity test of GEMS VCDs to a prior profiles

	WRF-Chem+CAM-Chem [WC]	GEOS-Chem [GC]
Resolution	28km x 28km, 69 layers	0.25º x 0.3125º, 47 layers
Target year	2016	2020
Anthropogenic emission	EDGAR-HTAP (2010)	KORUSv5 (2016)
Meteorological data	GFS 6 hourly 1 degree	GEOSFP 0.25º x 0.3125º

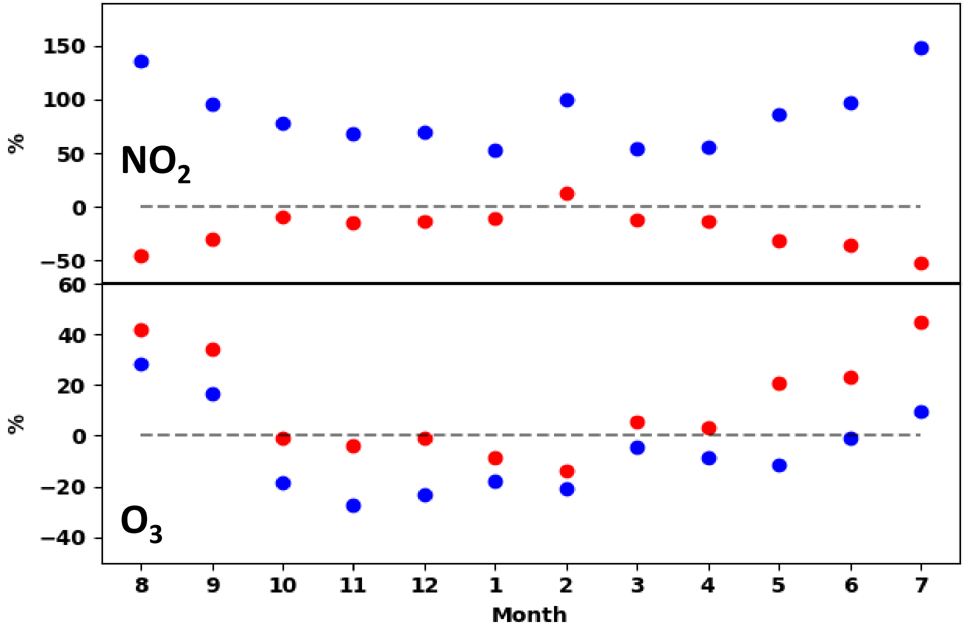
Compare with in-situ observation

Correlation coefficient



* : p-value > 0.05

Normalized mean bias



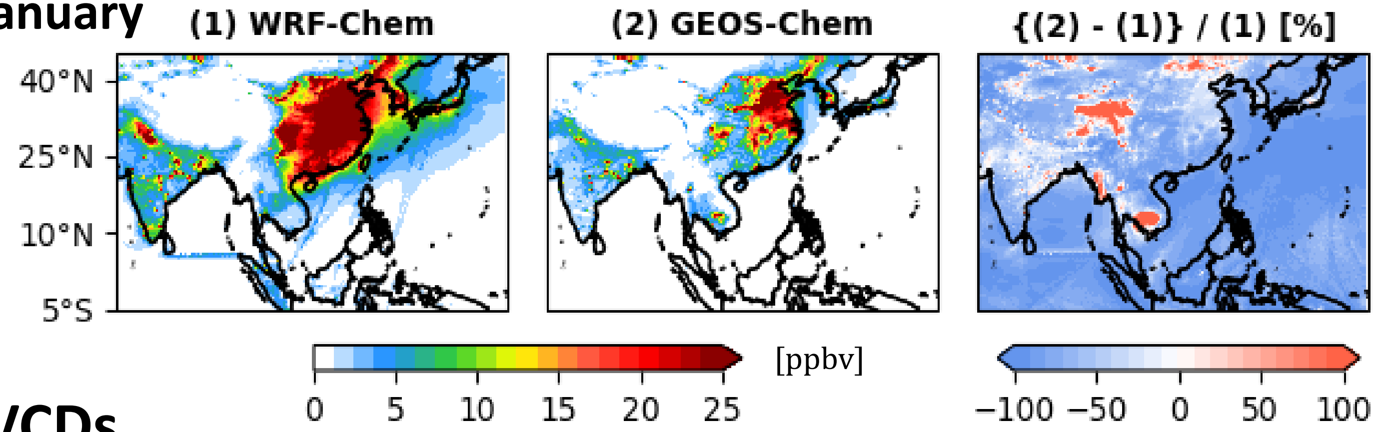
\# of observation :
China - 1600
South Korea - 549

ACMG

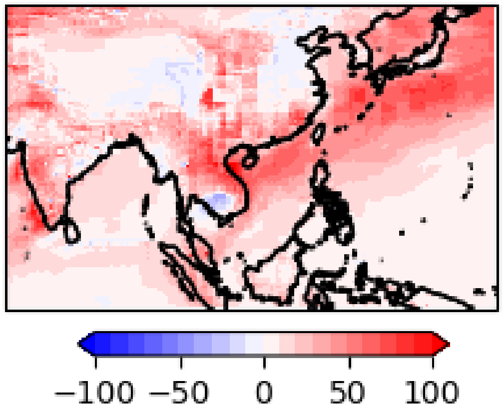
NO_2 VCDs change caused by a priori profile replacement

Surface mixing ratio difference

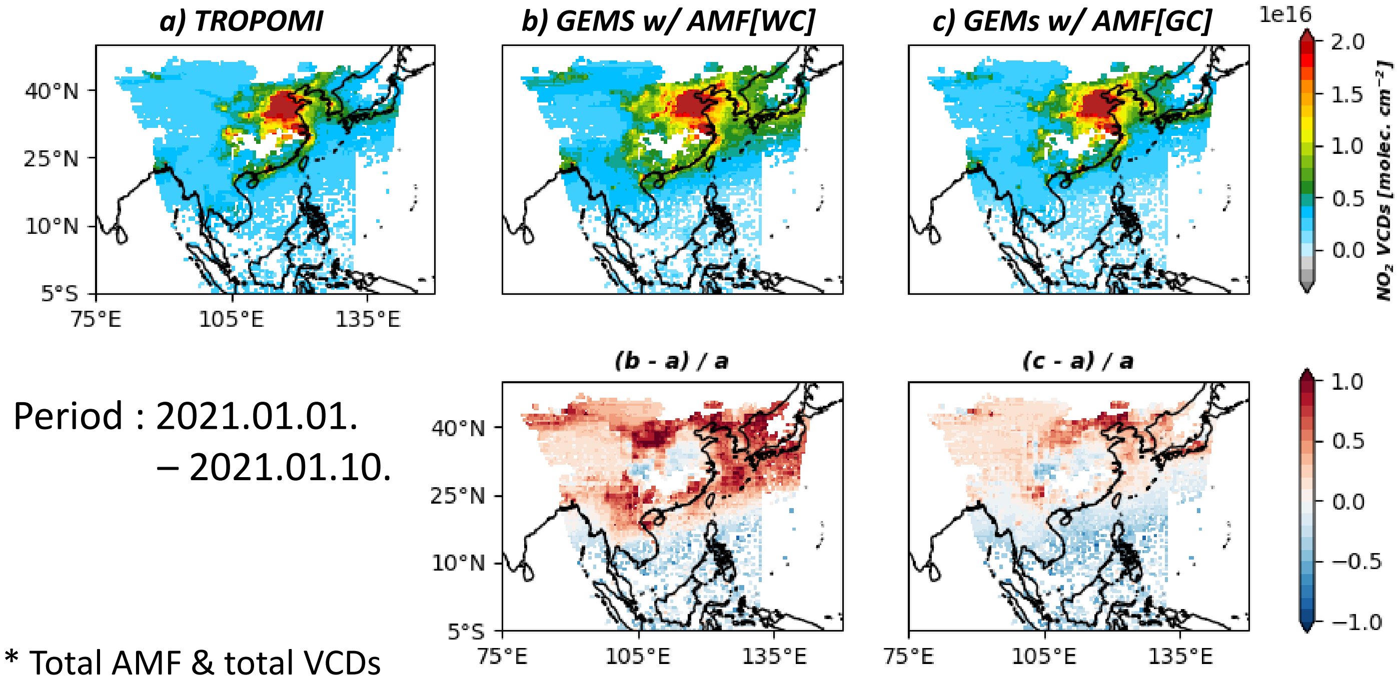
January



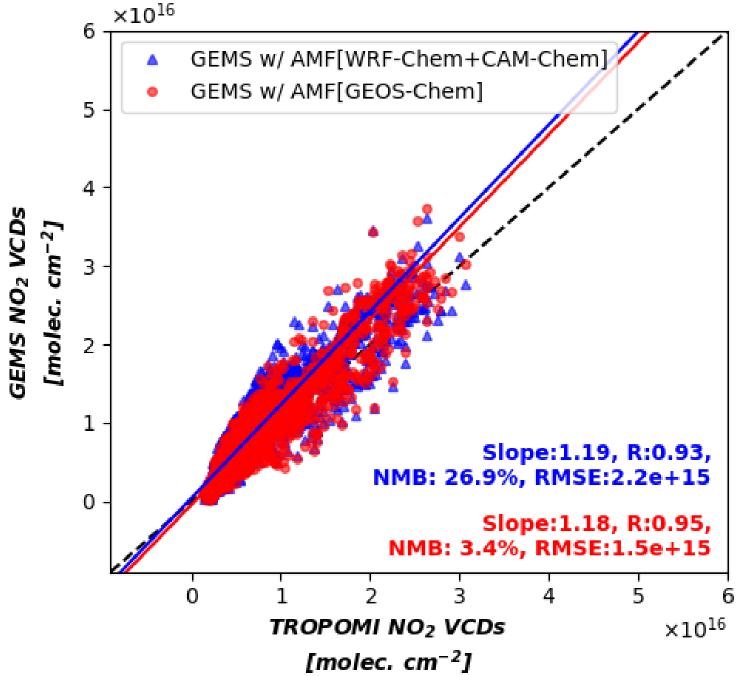
$$\left\{ \left(\frac{AMF[GC]}{AMF[WC]} \right) - 1 \right\} \times 100 \ [\%]$$



NO_2 VCDs



Period : 2021.01.01.
– 2021.01.10.

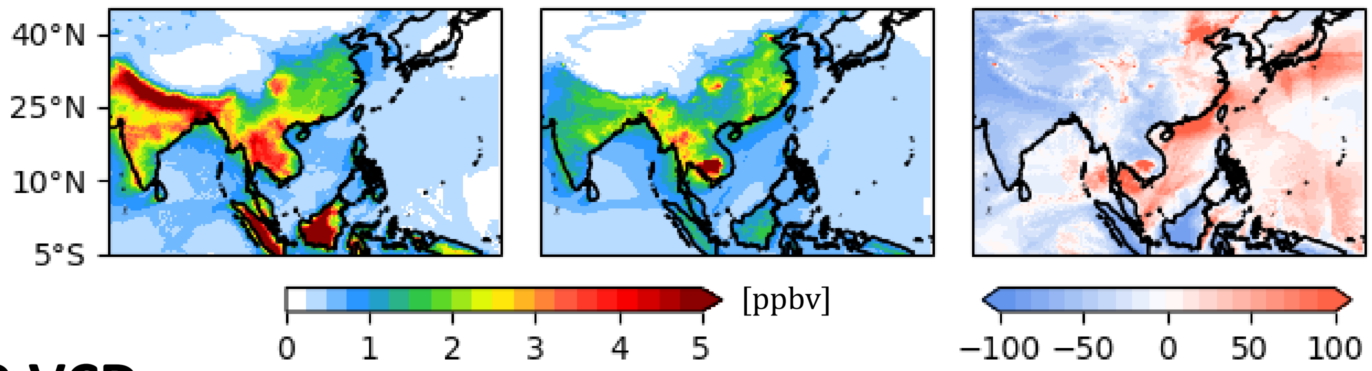


* Total AMF & total VCDs

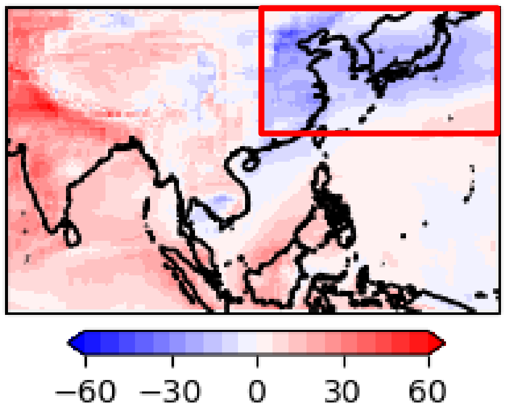
HCHO VCDs change caused by a priori profile replacement

Surface mixing ratio difference

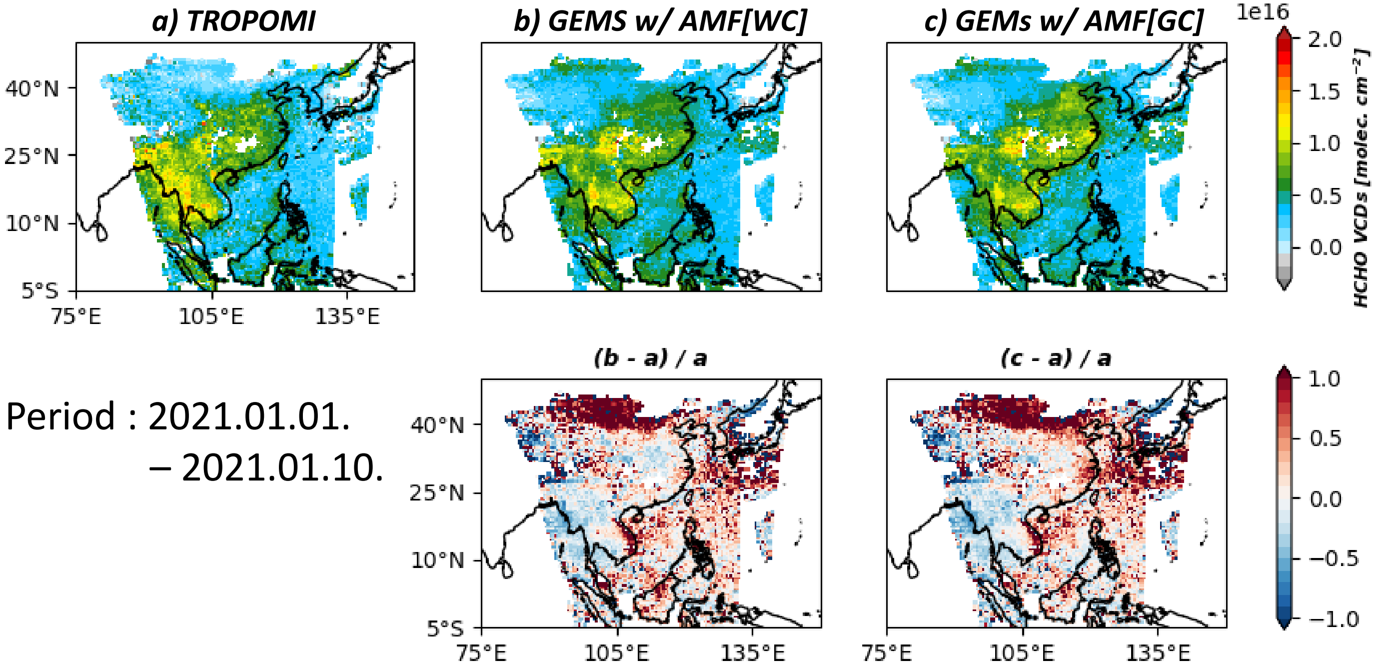
January



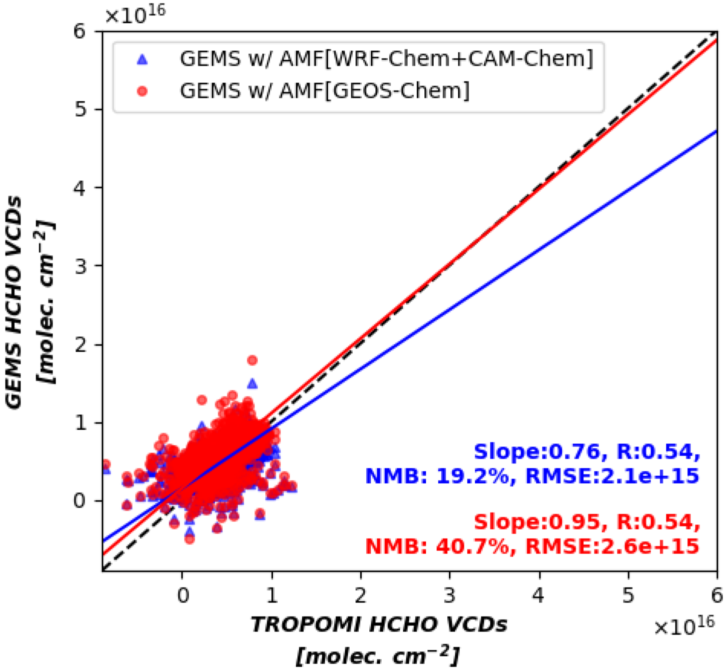
$$\left\{\left(\frac{AMF[GC]}{AMF[WC]}\right)-1\right\}\times 100\ [\%]$$



HCHO VCDs



Period : 2021.01.01.
– 2021.01.10.

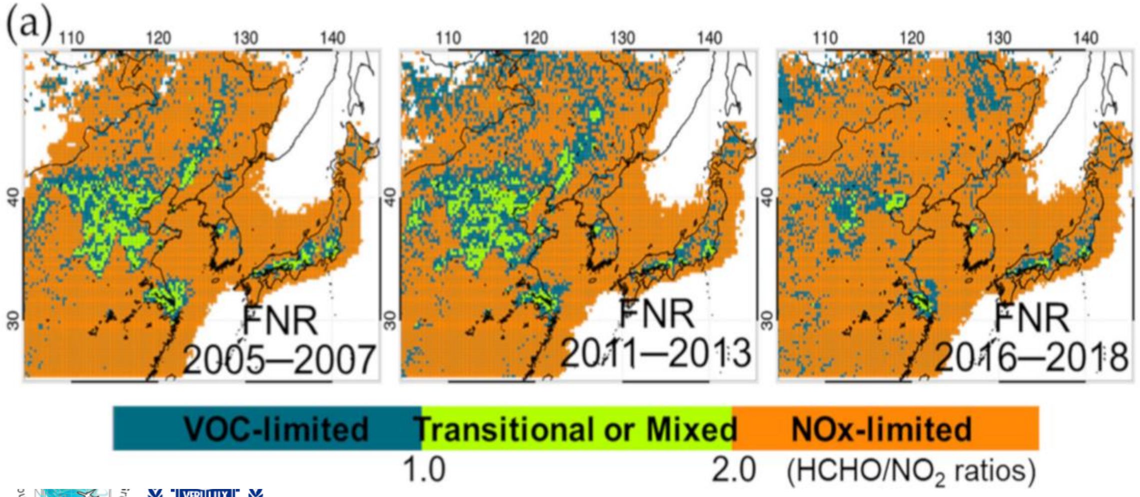


Diurnal variation: GEMS $HCHO/NO_2$ ratio

*** Preliminary results**

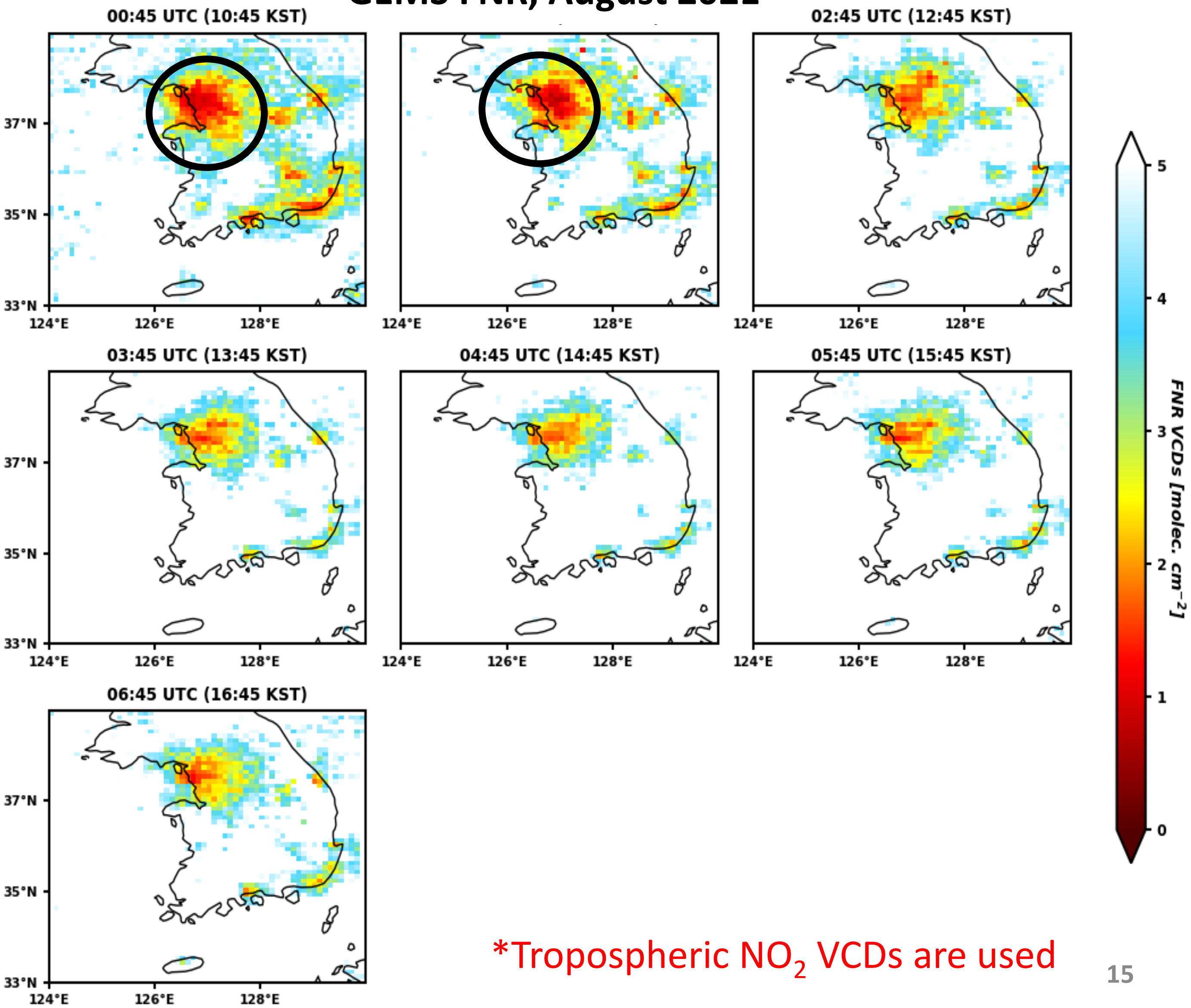
- **Formaldehyde to Nitrogen dioxide Ratio (FNR)**
  - Used to distinguish surface ozone formation mechanism
  - $FNR = \frac{HCHO}{NO_2}$
    - ✓ 0~1 (VOCs-limited)
    - ✓ 1~2 (Mixed)
    - ✓ 2~ (NOx-limited)

→ Simultaneous reductions of VOCs, NOx are necessary to mitigate the surface ozone production. [Oak *et al.*, 2019]



[Lee *et al.*, 2014]

GEMS FNR, August 2021

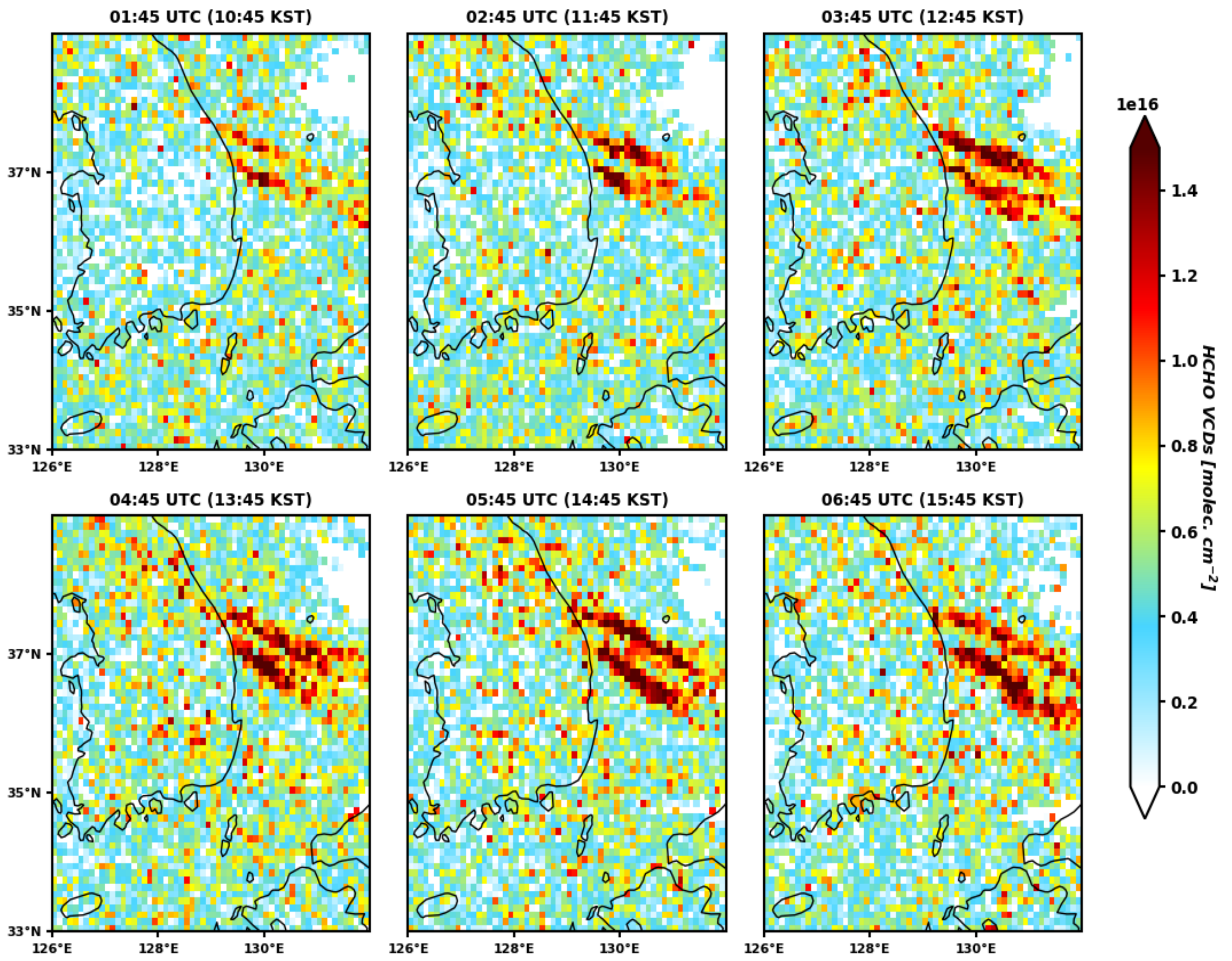


*Tropospheric NO_2 VCDs are used

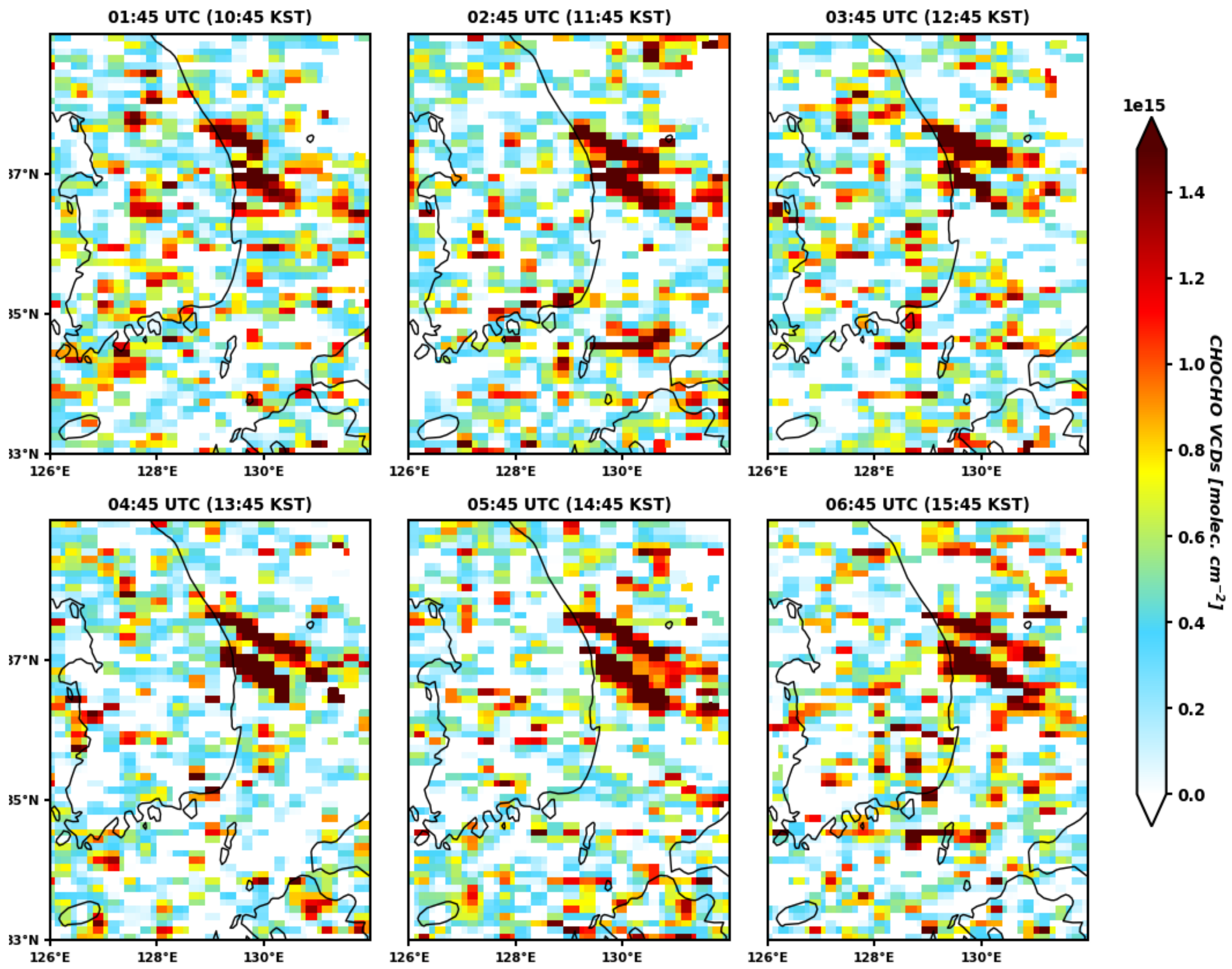
Uljin wildfire case study

* Preliminary results

GEMS HCHO, 2022.03.05.



GEMS CHOCHO, 2022.03.05.



- The wildfire has been well captured by GEMS with hourly daytime observations.

Top-down estimates of AVOC emissions

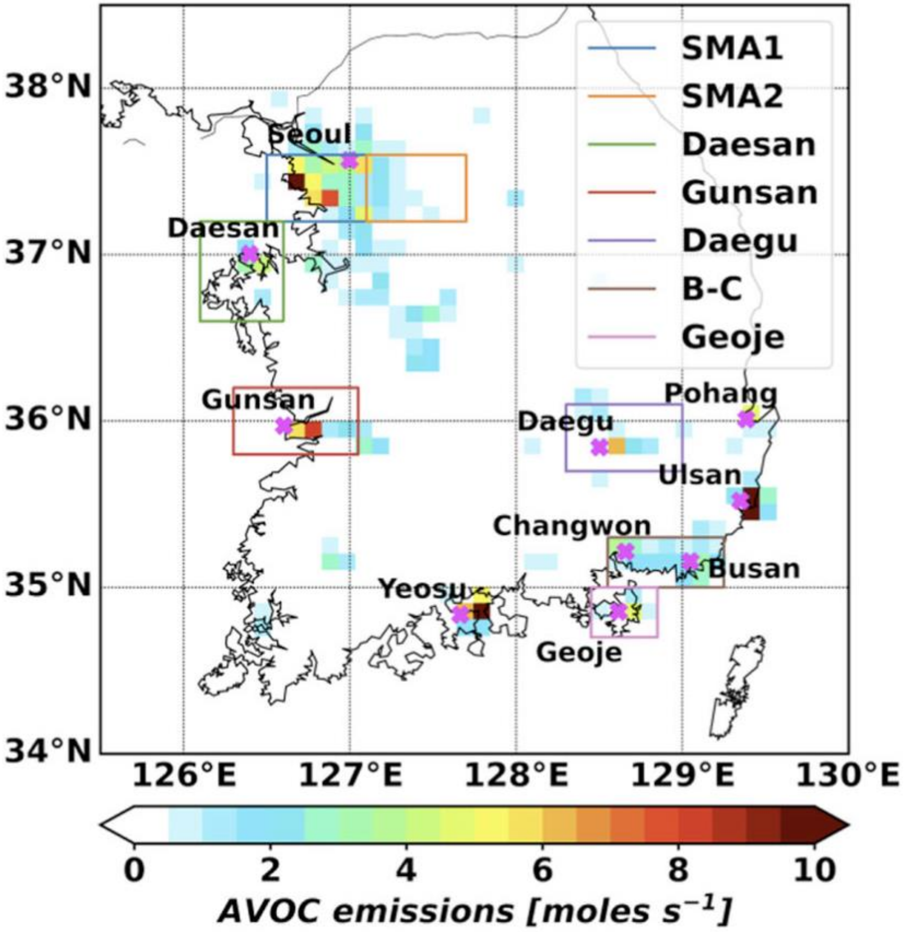
- S : total HCHO net production rate [kmol/h]

$$S = \frac{1}{\tau_{HCHO}} \oint \boxed{(\mathrm{VCD} - \mathrm{VCD}_0)} \mathrm{dA}$$

- E : total AVOC emissions [kmol/h]

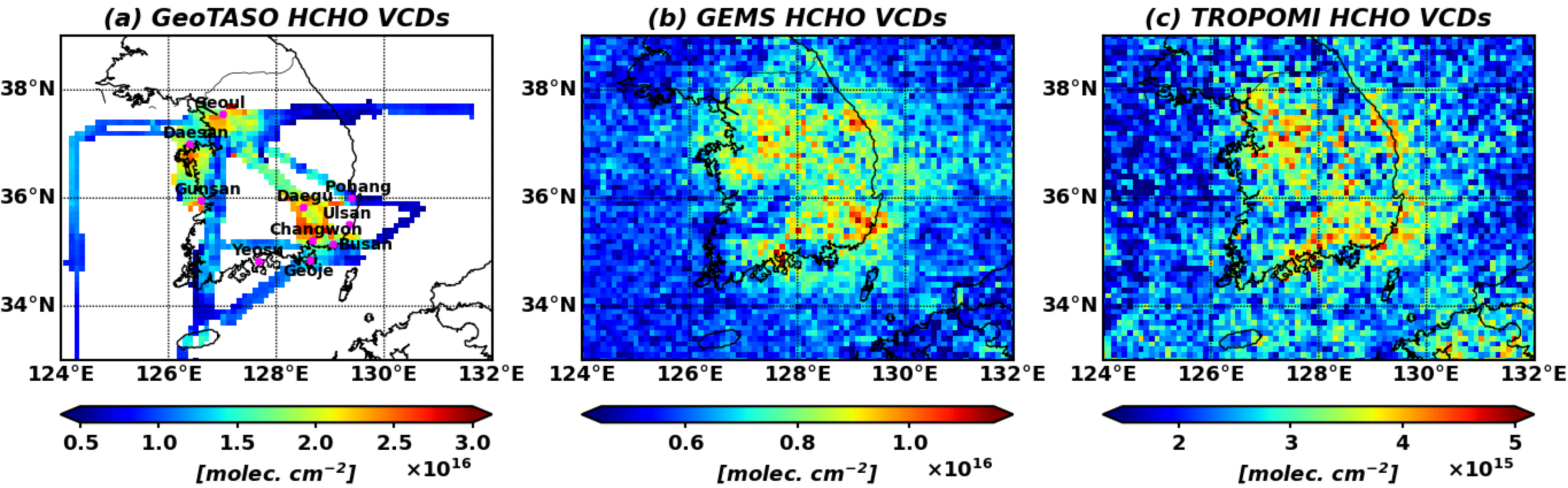
$$E = \frac{S}{\sum_i f_i Y_i}$$

f_i : emission fraction for species i
Y_i : HCHO yields for species i



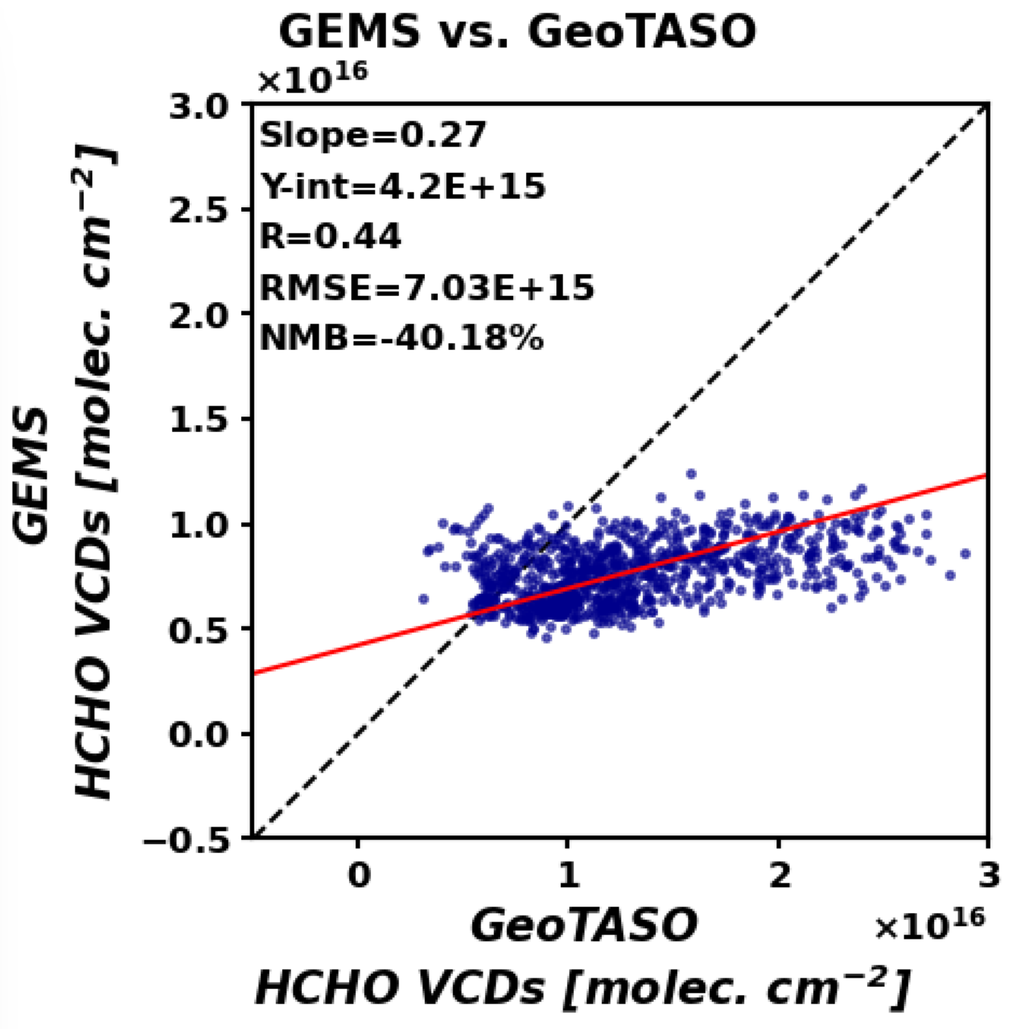
(Kwon et al., 2021)

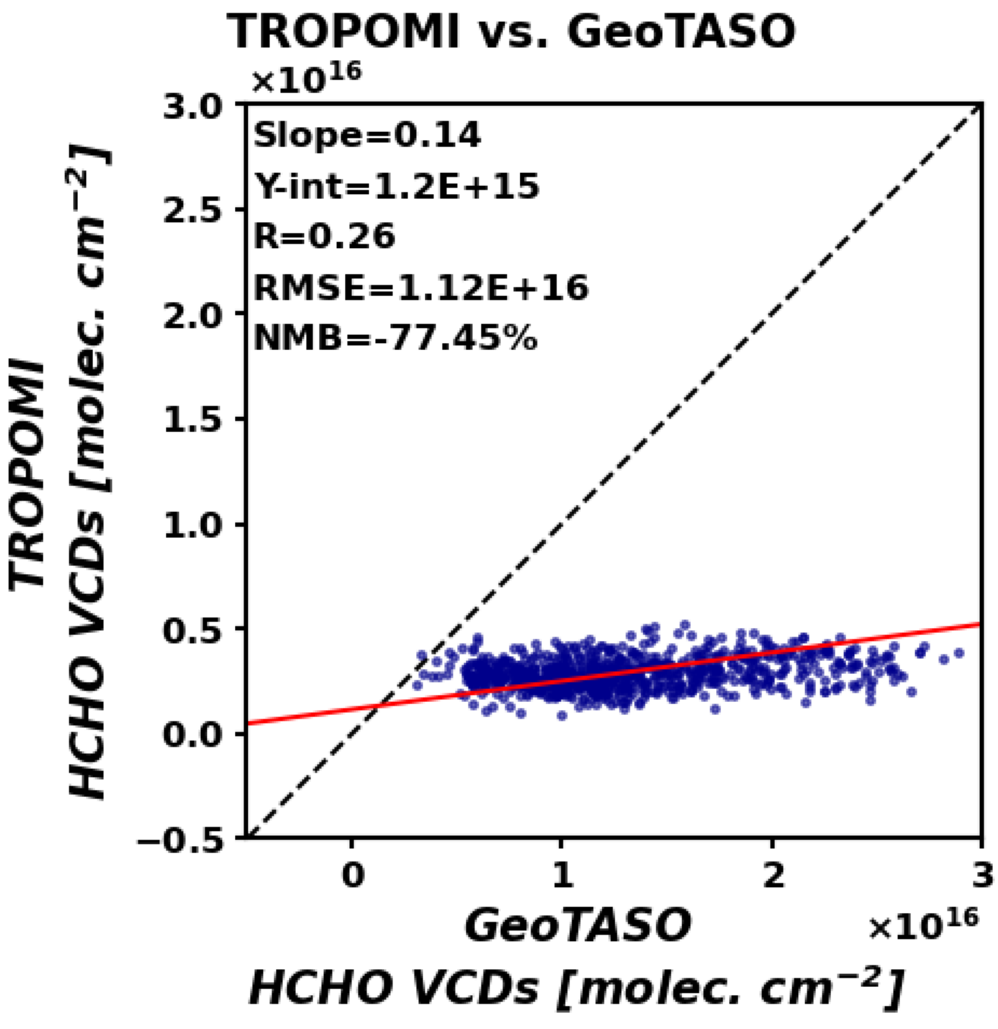
Comparison with airborne measurement



Year: 2016 Year: 2021 Year: 2021

Airborne measurement vs. Satellites





- Zhu et al. (2020) showed negative biases (−45 ~ −22%) of OMI HCHO under high-HCHO conditions compared to observations from 12 aircraft campaigns

Correction of GEMS VCDs by comparison with FTIR VCDs

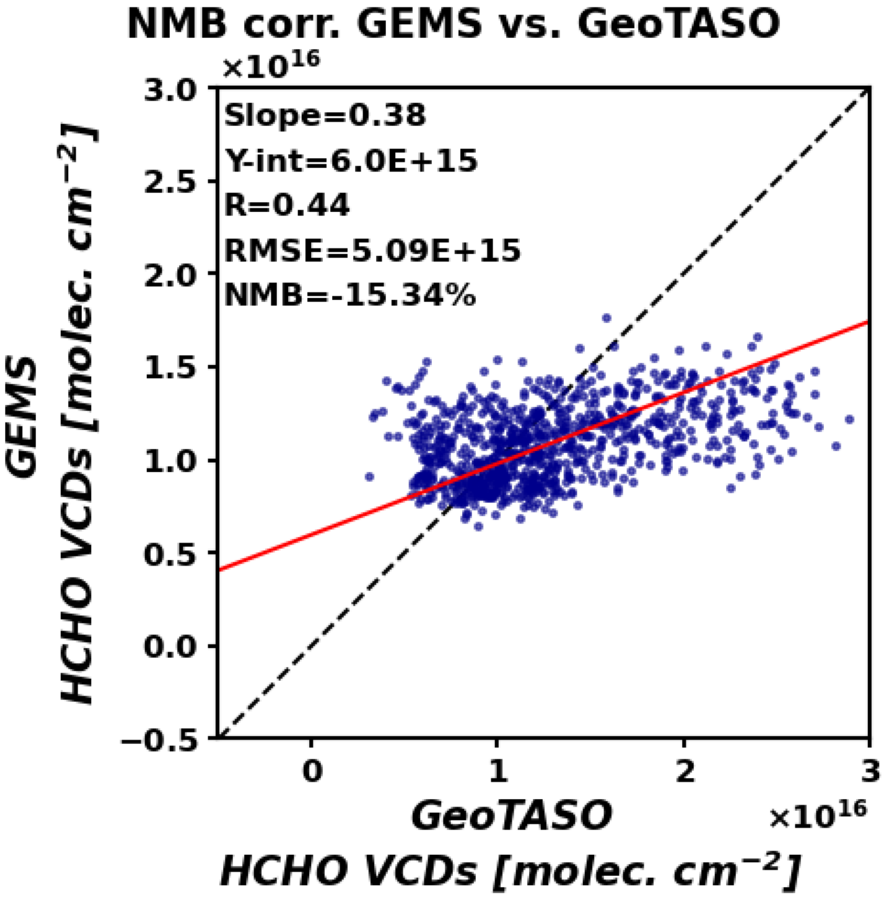
NMB = -29.34 %
slope = 0.55
y intercept = 1.6×10^{15}

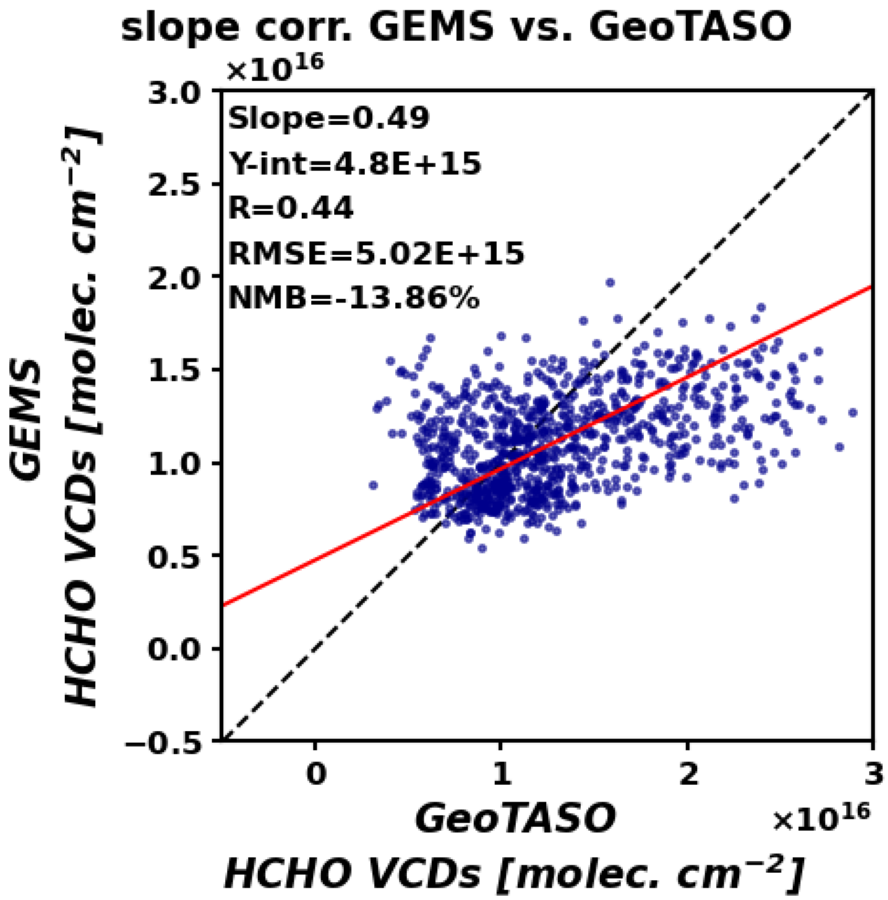
[Correction by NMB]

$$corrected\ VCD = \frac{1}{1 + NMB} \times\ VCD$$

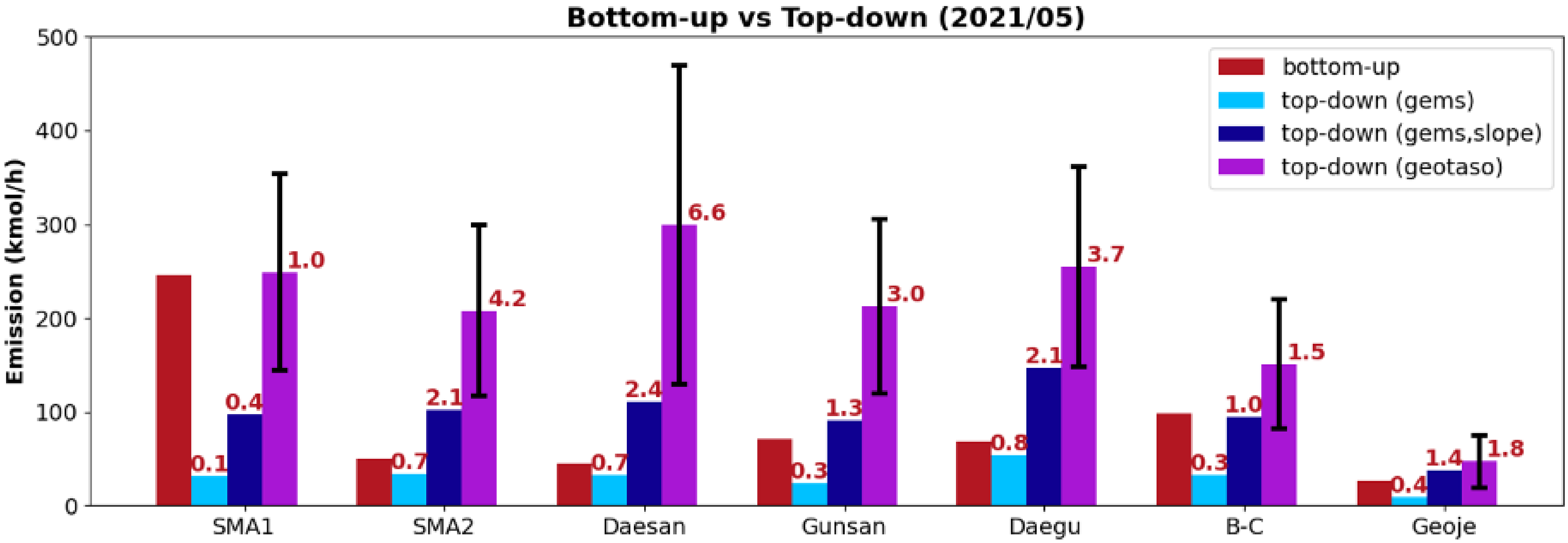
[Correction by slope]

$$corrected\ VCD = \frac{VCD\ - y\ intercept}{slope}$$





Top-down estimates of AVOC emissions: GEMS vs. Geo-TASO

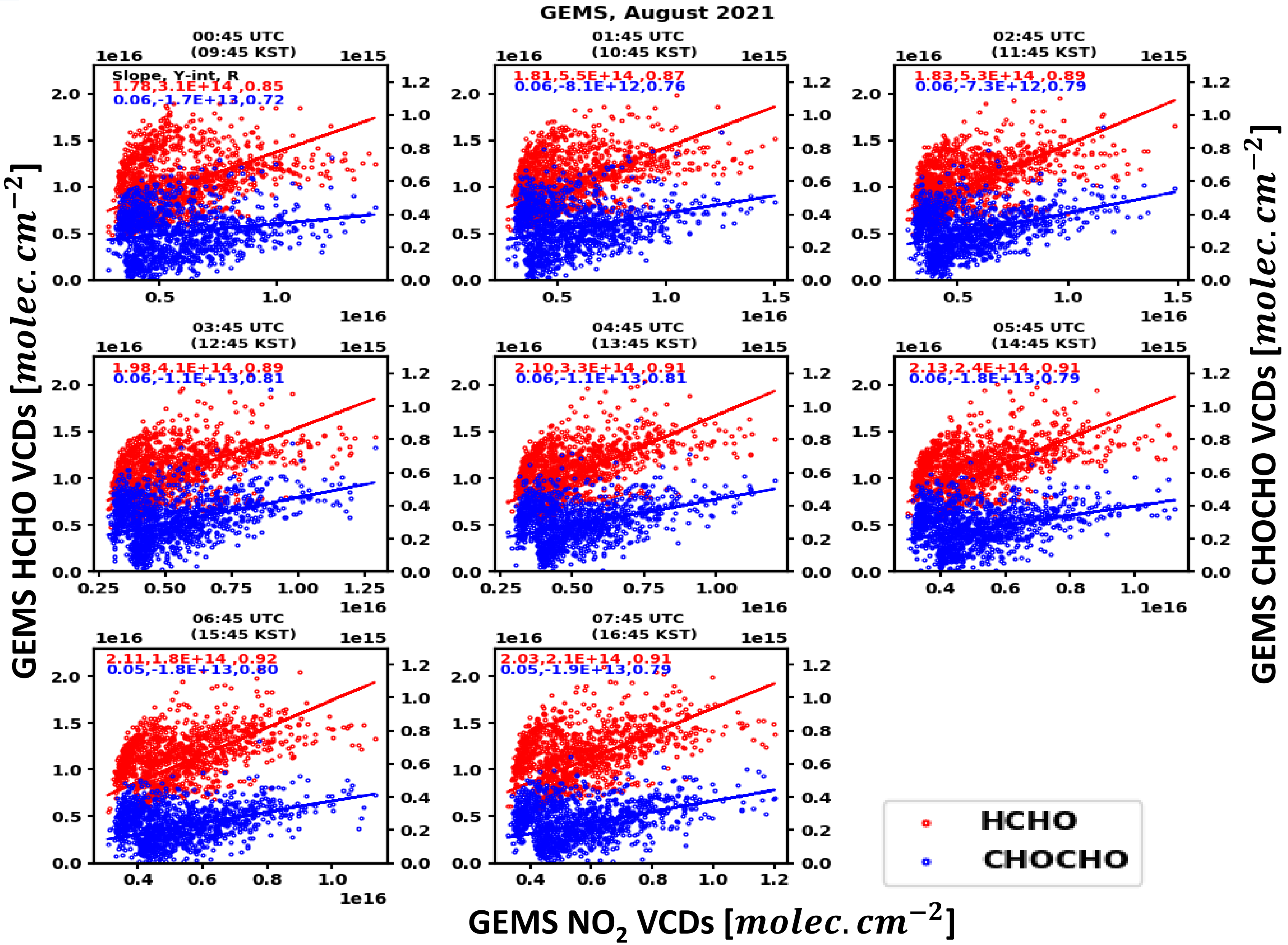


- Bottom-up emission: KORUS V5 inventory
- $VCD_0 = 6.3 \times 10^{15}$: Average HCHO VCD over the background area from GeoTASO and GEOS-Chem *(Kwon et al, 2021)*

Thank you for your attention

Correlations of NO_2 with HCHO and CHOCHO in GEMS observation

* Preliminary results



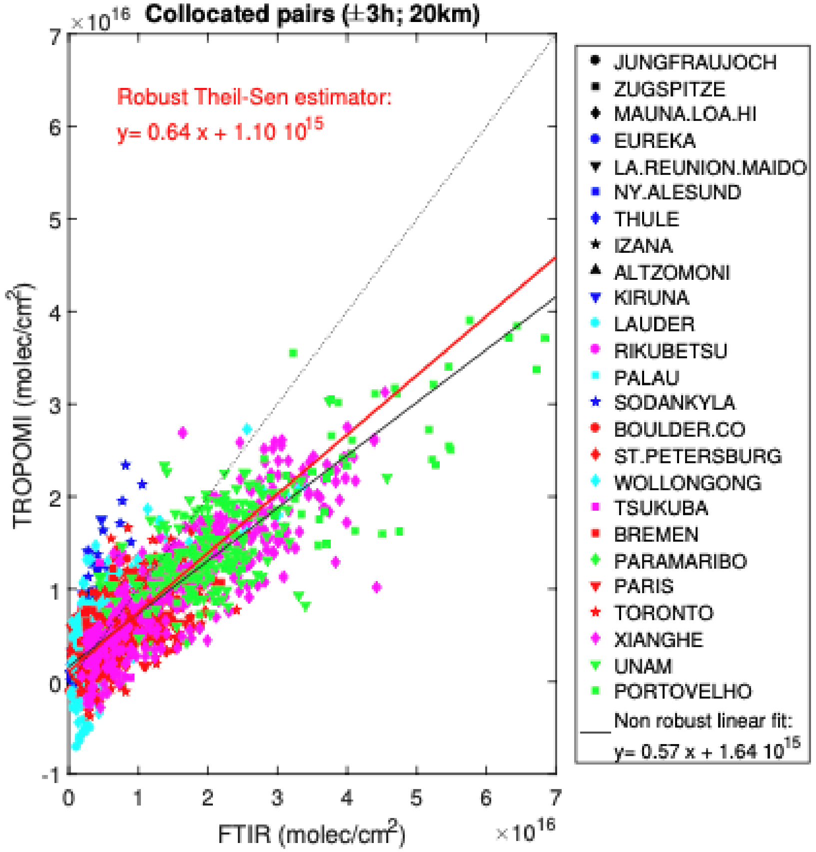
Bias dependency on HCHO concentration

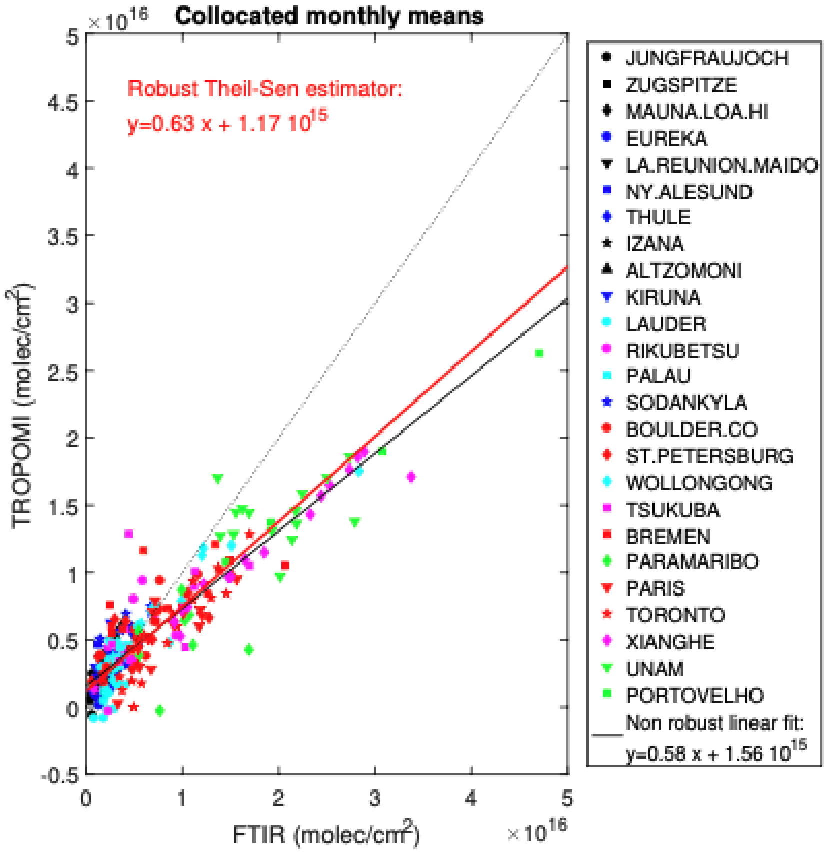
- Bias of TROPOMI HCHO w.r.t. FTIR *(Vigouroux et al., 2020)*

✓ Negative biases (-30.8%±1.4%) under high-HCHO conditions (>8.0×10^{15} molec/cm^2)

✓ High biases (26%±5%) under low-HCHO conditions (<2.5×10^{15} molec/cm^2)

  - The biases can be used, e.g., to correct TROPOMI data near emission sources.





Comparison of HCHO and CHOCHO VCDs: GEMS vs. GEOS-Chem

Period : 2021.05.01 ~ 2021.06.30