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## Validation of GEMS operational v2.0 total column NO<sub>2</sub> and HCHO during the GMAP/SIJAQ campaign

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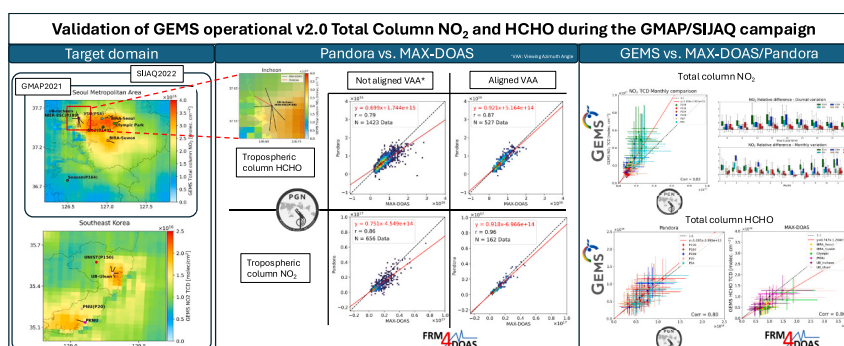
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### HIGHLIGHTS

- A comparative analysis of MAX-DOAS and Pandora was investigated.
- GEMS total column NO<sub>2</sub> and HCHO was validated using Pandora and MAX-DOAS measurements in South Korea.
- A significant overestimation of GEMS NO<sub>2</sub> data was observed, particularly in urban areas like Seoul, compared to rural areas.
- A systematic underestimation of GEMS HCHO total column product was observed, particularly in large columns.

### GRAPHICAL ABSTRACT



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## ABSTRACT

The Geostationary Environmental Monitoring Spectrometer (GEMS), the first geostationary air quality instrument, onboard the GEO-KOMPSAT-2B (GK2B) satellite, produces hourly observations over Asia with 3.5 km × 8 km spatial resolution. To evaluate the GEMS L2 products, the National Institute of Environmental Research (NIER) organized the GEMS Map of Air Pollutants 2021 (GMAP2021) and the Satellite Integrated Joint monitoring of Air Quality 2022 (SIJAQ2022) campaigns during October 2021 to November 2021 and from June 2022 to July 2022, respectively. While GMAP2021 mainly targeted the SMA (Seoul Metropolitan Area), the SIJAQ2022 campaign extended to the southeastern area of South Korea. In this study, a comparison between Pandora and Multi-Axis Differential Optical Absorption Spectroscopy (MAX-DOAS) products and an evaluation of the GEMS operational v2.0 total column NO<sub>2</sub> and HCHO products are conducted.

A comparative analysis between the Pandora (P189) and the IUP Bremen MAX-DOAS instrument at the Incheon NIER-ESC site was performed to analyze discrepancies between the retrieval processors (Pandora: PGN official processor, MAX-DOAS: MMF in FRM<sub>4</sub>DOAS framework). Aligning the viewing directions of both Pandora and MAX-DOAS leads to a significant increase in the slope and correlation coefficient from 0.87 to 0.96 and from 0.86 to 0.96, respectively, in the case of NO<sub>2</sub> tropospheric columns. Similarly, for HCHO tropospheric columns, slope and correlation coefficient change from 0.94 to 1.09 and from 0.81 to 0.90 when matching the viewing geometries of both instruments. In contrast to tropospheric columns, total HCHO columns derived from Pandora (P189) direct-sun measurements show significantly larger values than the MAX-DOAS ones, with a mean relative difference (MRD) of 126 %. This bias can however be reduced to 33 % after suitable adjustment of the direct-sun retrieval settings.

The GEMS v2.0 NO<sub>2</sub> total column product, evaluated over 6 official PGN sites in South Korea, shows good agreement with a correlation coefficient of 0.87 and similar seasonal and diurnal NO<sub>2</sub> variation. However, GEMS tends to report higher values than Pandora with a mean relative difference of +41 %. The magnitude of the GEMS overestimation is amplified in highly polluted conditions (i.e. during winter and at noontime).

Compared to 6 MAX-DOAS stations and 6 Pandora stations, the GEMS HCHO product captures well the seasonal and diurnal variation of HCHO and shows good agreement both with MAX-DOAS and Pandora with slopes of 0.84 and 0.79, respectively, and correlation coefficients of 0.86 for both. Large columns, however, tend to be systematically underestimated.

## 1. Introduction

Nitrogen oxides (NO<sub>x</sub> = NO + NO<sub>2</sub>) are key species for air quality research due to their toxicity and significant role in atmospheric chemistry. NO<sub>x</sub> is mainly emitted as NO, which quickly converts to NO<sub>2</sub> by reacting with ozone (O<sub>3</sub>). NO<sub>x</sub> is naturally emitted from sources such as soil, lightning, and natural biomass burning. In recent decades, the emissions of NO<sub>x</sub> have dramatically increased due to anthropogenic sources including domestic heating (Schiavon et al., 2015; Ozgen et al., 2021), power plants (Kim et al., 2006; Saw et al., 2021), transportation (Jaegle et al., 2005; Kousoulidou et al., 2008), and industrial activities (Van Der et al., 2008). High-concentrations of NO<sub>2</sub> directly cause respiratory diseases such as asthma, lung cancer, and cardiopulmonary condition (Elsayed, 1994; Eum et al., 2022) and it contributes to the formation of particulate matter (PM) (Behera and Sharma, 2011; Chu et al., 2020). In addition, NO<sub>2</sub> is a key component controlling ozone production through reactions involving Volatile Organic Compounds (VOCs) (Crutzen, 1979; Haagen-Smit, 1952). Due to its high reactivity, the lifetime of NO<sub>2</sub> in the lower atmosphere is only a few hours (Laughner and Cohen, 2019).

Formaldehyde (HCHO) is another important trace gas in atmospheric chemistry. HCHO is an intermediate product of the VOCs oxidation and can be considered as a tracer of VOCs (Li et al., 2014; Lui et al., 2017). The background concentration of HCHO mainly results from the oxidation of methane (CH<sub>4</sub>) (González Abad et al., 2016) but higher concentrations are found over continents due to direct emissions from industrial sources as well as the oxidation of non-methane volatile organic compounds (NMVOCs) emitted by human activity and biogenic sources (Dutta et al., 2010). HCHO is a carcinogen, and can cause inspiratory diseases and headaches (EPA, 2015; Zhu et al., 2017a). Furthermore, HCHO is a key reactant in tropospheric ozone chemistry, as photochemical reactions produce hydroperoxyl radicals (HO<sub>2</sub>), which subsequently reacts with nitric oxide (NO) to produce hydroxyl radicals (OH). Due to its high reactivity, the lifetime of HCHO is just a few hours in the atmosphere (De Smedt et al., 2008).

Due to their short lifetimes, the spatial distributions of both NO<sub>2</sub> and HCHO are closely related to the location of their emission sources, which has been used to estimate emission fluxes (Beirle et al., 2011; de Foy et al., 2015; Ghude et al., 2008; Gonzi et al., 2011). Space-borne instruments such as the Global Ozone Monitoring Experiment (GOME; Burrows et al., 1999 and GOME-2; Munro et al., 2006), the Scanning Imaging Absorption spectrometer for Atmospheric Cartography (SCIAMACHY; Bovensmann et al., 1999), the Ozone Monitoring Instrument (OMI; Levelt et al., 2006), the Ozone Mapping and Profiler Suite (OMPS; Flynn et al., 2006) and the Tropospheric Monitoring Instrument (TROPOMI; Veeffkind et al., 2012), all operated on polar orbit satellites (Low-Earth Orbit; LEO), have been used since the mid-nineties providing valuable information on NO<sub>2</sub> and HCHO spatial distributions and trends with full-earth coverage (Richter et al., 2005; Schneider et al., 2015; Van Der et al., 2006; Zhu et al., 2017b). Since they overpass a target region in mid latitudes only once or twice a day at best, LEO satellites are limited in their temporal coverage. To overcome this limitation and inform on the diurnal characteristics of atmospheric trace gas concentrations, Korea launched the first geostationary environmental monitoring satellite GEMS (Geostationary Environmental Monitoring Spectrometer) in 2020 (Kim et al., 2020). This was followed by the US TEMPO (Tropospheric Emissions: Monitoring of Pollution) mission launched in 2023 (Zoogman et al., 2017) and, in 2025, the European Space Agency (ESA) will launch the Copernicus Sentinel-4 instrument (Gulde et al., 2017).

For the validation of GEMS measurements, the National Institute of Environmental Research (NIER) has been expanding the Pandora network over Asia by organizing the PAN (Pandora Asia Network). Furthermore, NIER organized two successive international field campaigns GMAP (GEMS Map of Air Pollution) and SIJAQ (Satellite Integrated Joint monitoring of Air Quality) during autumn 2021 and summer 2022.

Kim et al. (2023) evaluated the GEMS operational v1.0 NO<sub>2</sub> vertical column density (VCD) products using four Pandora instruments from November 2020 to January 2021 in Seosan, Korea. This study reported that the GEMS v1.0 NO<sub>2</sub> VCD product was lower than Pandora

observations and showed correlation coefficients of 0.62–0.78. Lange et al. (2024) evaluated the tropospheric NO<sub>2</sub> VCD from the GEMS operational v2.0 processor and the IUP-UB scientific product using Pandora and MAX-DOAS data during the GMAP and SIJAQ campaigns. The GEMS operational product overestimated ground-based instruments by a median relative bias of 64 % with a correlation coefficient of 0.75. In contrast, the IUP-UB scientific product showed a median relative bias of –1 % with a correlation coefficient of 0.82. This study found that urban areas exhibit maximum NO<sub>2</sub> columns around 11 LST, while rural areas show nearly no diurnal variability. Lee et al. (2024) conducted the first evaluation of the GEMS operational v2.0 HCHO product using Fourier-Transform Infrared (FTIR) and Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) from October 2020 to January 2021 in Xianghe, China. They found that the GEMS HCHO product was 30–40 % lower than MAX-DOAS and FTIR observations, likely due to differences in vertical sensitivity between the instruments. Applying an averaging kernel smoothing method reduced this low bias by about 10–15 %. Nevertheless, GEMS effectively captured the seasonal variability of HCHO over East Asia.

In sections 2 and 3, we briefly introduce the GMAP and SIJAQ campaigns conducted over Korea, as well as the satellite and ground-based remote sensing data used in this study. In section 4, focusing on the NIER-ESC site, comparison results of NO<sub>2</sub> and HCHO retrievals obtained by MAX-DOAS and Pandora instruments are presented. The validation of GEMS operational v2.0 NO<sub>2</sub> and HCHO total column products using Pandora and MAX-DOAS instruments operated over Korea is reported in Section 5.

## 2. GMAP/SIJAQ campaigns

The GMAP/SIJAQ campaigns are a set of field campaigns organized in Korea by NIER. One of their main objectives was to perform intensive field measurements to produce a reference data set for validating the GEMS retrieval products based on surface in-situ, in-situ aircraft, airborne remote sensing, car DOAS, and stationary remote sensing observations. The GMAP2021 campaign (<https://www.sijaq.org/home>, last access: 25 March 2024) took place from October 2021 to November 2021 over the Seoul Metropolitan Area (SMA). Subsequently, from June 2022 to August 2022, the SIJAQ2022 campaign (<https://sijaq2.sijaq.org/>, last access: 25 March 2024) was conducted by expanding the target domain to the southeastern area of Korea which includes the cities of Busan and Ulsan.

In the beginning of the GMAP2021 campaign, early October 2021, the Royal Belgian Institute for Space Aeronomy (BIRA-IASB), the Institute of Environmental Physics, University of Bremen (IUP Bremen), and the Max Planck Institute for Chemistry (MPIC) installed three MAX-DOAS instruments at the rooftop of NIER-ESC for one week intercomparison, before each instrument moved to a different observation site (BIRA\_Suwon, UB\_Incheon, MPIC\_Olympic, respectively, see Table 1). Details on the intercomparison experiment can be found in Van Roozendaal et al. (2024). UB\_Incheon and MPIC\_Olympic sites were

continuously operated until mid-November 2022 and early August 2022, respectively. BIRA-IASB operated the BIRA-Suwon station during the GMAP2021 campaign period, then moved to the BIRA-Seoul site from December 2021 to June 2022. For SIJAQ2022, IUP Bremen and MPIC installed additional MAX-DOAS instruments at UB\_Ulsan and MPIC\_PKNU in Ulsan and Busan respectively. In addition to the MAX-DOAS instruments from the European groups, 6 official PGN Pandora stations were also involved in the campaign. Furthermore, NIER installed two additional non-PGN Pandora instruments. To ensure optimal consistency, this study only uses official data that were calibrated and processed by the PGN processors. The location and information of all sites used in this study are described in Fig. 1 and Table 1. The operational periods of each instrument are illustrated in Fig. A.1 and the observation schedule of GEMS can be found in Fig. A.2.

## 3. Instruments

### 3.1. MAX-DOAS

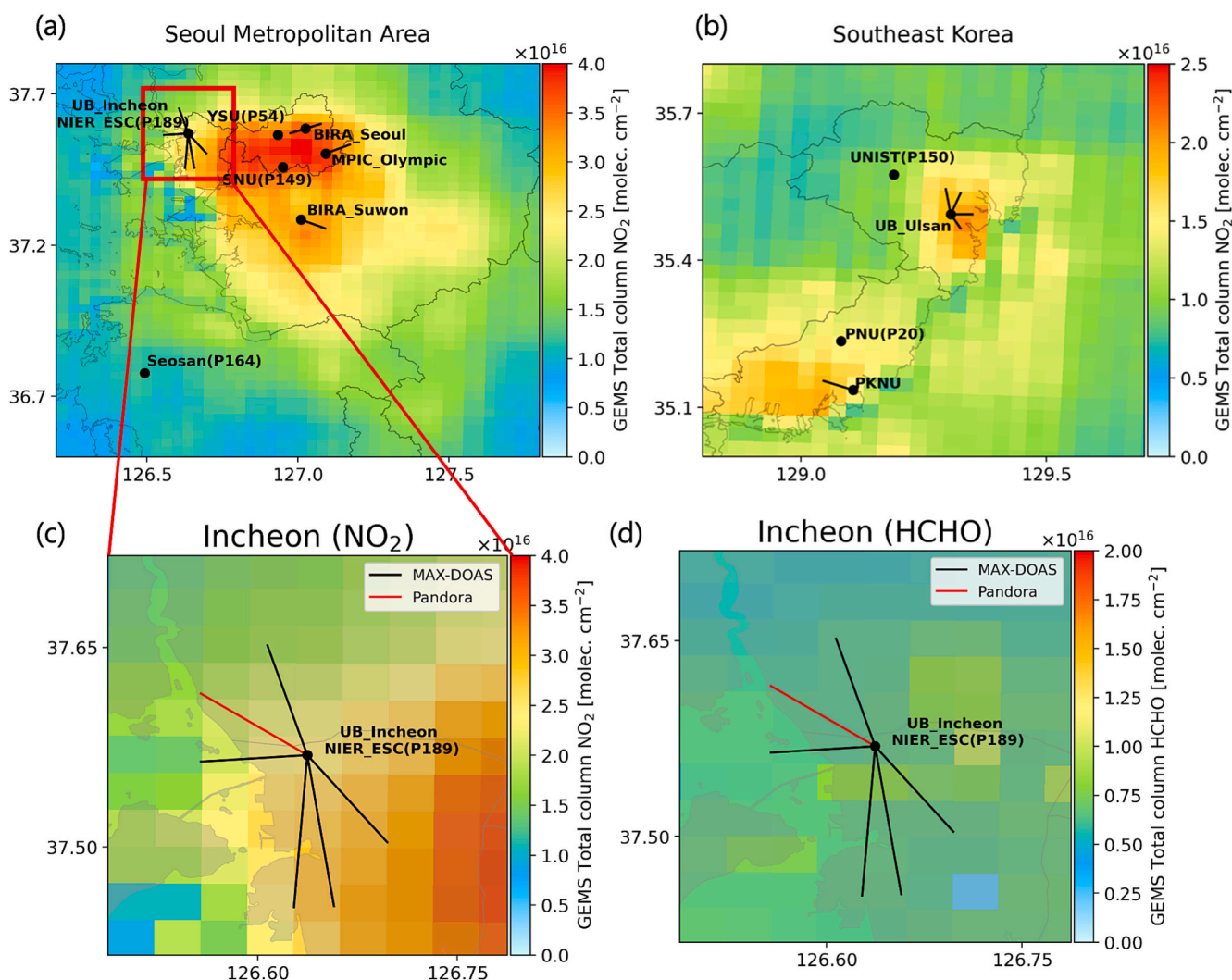
The Multi-axis Differential Optical Absorption Spectroscopy (MAX-DOAS) is a ground-based remote sensing technique used for observing trace gases in the atmosphere such as NO<sub>2</sub>, SO<sub>2</sub>, and HCHO (Hönninger et al., 2004). MAX-DOAS instruments conduct vertical scanning at multiple elevation angles from 0° to 90°. In general, NO<sub>2</sub> and HCHO profiles can be reliably retrieved from near the ground up to approximately 2 km altitude. Vertical columns are representative of the column between the surface and 4 km of altitude (Irie et al., 2011; Tirpitz et al., 2021). The differential slant column densities (dSCDs) are fitted from a set of off-axis spectra and a corresponding reference zenith spectrum. The dSCDs are converted to VCDs by applying the Air Mass Factor (AMF) (Platt and Stutz, 2008). In this campaign, we processed spectra obtained from each instrument using first QDOAS (Danckaert et al., 2017) to get the dSCD and then the Mexican MAX-DOAS Fit (MMF; Friedrich et al., 2019) algorithm for retrieving tropospheric VCDs. The analysis was performed using the centralized FRM<sub>4</sub>DOAS framework (<https://frm4doas.aeronomie.be>, last access: 12 March 2024). The quality flagging of MMF as implemented in the FRM<sub>4</sub>DOAS framework takes into account the degree of freedom (DOF) of the retrieval, the root mean square (RMS) of the difference between measured and simulated dSCD and a stability criterion based on using different a priori values for the aerosol retrieval. Three quality flag values are possible: 2 (quality check failed), 1 (warning) and 0 (ok). The FRM<sub>4</sub>DOAS framework provides quality flags independently from both the MMF and Mainz profile algorithm (MAPA, Beirle et al., 2019), as well as an overall quality flag by combining the quality flags from both algorithms. In our analysis, we only consider MMF retrieved data filtered with overall quality flags (qa\_flag\_no2 and qa\_flag\_hcho) of 0 and 1.

### 3.2. Pandora

The Pandora instrument is a hyperspectral UV–visible ground-based

**Table 1**  
Geolocation information and observation period of stationary instrument sites.

| Instrument | Station      | Affiliation | Location                        | Period                |
|------------|--------------|-------------|---------------------------------|-----------------------|
| MAX-DOAS   | BIRA_Seoul   | BIRA-IASB   | Seoul (127.026° E, 37.585° N)   | 2021.12.19–2022.06.02 |
| MAX-DOAS   | BIRA_Suwon   | BIRA-IASB   | Suwon (127.010° E, 37.284° N)   | 2021.10.21–2021.12.16 |
| MAX-DOAS   | UB_Incheon   | IUP-Bremen  | Incheon (126.638° E, 37.569° N) | 2021.10.09–2022.11.14 |
| MAX-DOAS   | UB_Ulsan     | IUP-Bremen  | Ulsan (129.306° E, 35.493° N)   | 2022.06.30–2022.11.13 |
| MAX-DOAS   | MPIC_Olympic | MPIC        | Seoul (127.093° E, 37.503° N)   | 2021.10.19–2022.08.05 |
| MAX-DOAS   | PKNU         | MPIC        | Busan (129.107° E, 35.135° N)   | 2022.06.17–2022.08.10 |
| Pandora 1S | P149         | SNU         | Seoul (126.951° E, 37.458° N)   | 2021.10.01–2022.11.30 |
| Pandora 1S | P150         | UNIST       | Ulsan (129.190° E, 35.575° N)   | 2021.10.01–2022.11.03 |
| Pandora 1S | P164         | NIER        | Seosan (126.494° E, 36.777° N)  | 2021.10.30–2022.11.30 |
| Pandora 1S | P189         | NIER        | Incheon (126.638° E, 37.569° N) | 2022.02.03–2022.11.30 |
| Pandora 1S | P20          | PNU         | Busan (129.083° E, 35.235° N)   | 2021.10.01–2022.11.30 |
| Pandora 1S | P54          | YSU         | Seoul (126.934° E, 37.564° N)   | 2021.10.01–2022.11.30 |



**Fig. 1.** Overview of the campaign domain and the location of stationary instruments over (a) the Seoul Metropolitan Area (SMA) and (b) the Southeast region. The background color represents the averaged GEMS total column  $\text{NO}_2$  from October 2021 to November 2022. The black dot represents the location of each ground-based remote sensing instrument station, and the black lines are the viewing directions of each MAX-DOAS. (c) is a zoomed-in view of the Incheon region (red box) in (a), with the viewing direction of the MAX-DOAS (black) and Pandora (red). (d) is the same as (c), but the background color represents the averaged GEMS total column HCHO for the same period.

instrument that has a 280 nm to 530 nm spectral range and 0.6 nm spectral resolution (Herman et al., 2009). It was developed by NASA to fill the lack of ground-based trace gas observations. The Pandora observation network is maintained by the Pandonia-Global-Network (PGN), which involves a collaboration between NASA and ESA. Measurement data from Pandora instruments are automatically transferred to the PGN server and are centrally processed through the Blick Software Suite to retrieve L2 products. Official products are available via the PGN data server (<https://data.pandonia-global-network.org/>, last access: 22 March 2024). In addition to total column (TCD) products derived from direct-sun measurements, PGN also retrieves tropospheric columns and surface concentrations from sky measurements, using a technique similar to the MAX-DOAS one. The retrieval algorithms for total and tropospheric columns of  $\text{NO}_2$  and HCHO are well described in Herman et al. (2009) and in Spinei et al. (2018), respectively. The HCHO TCD from Pandoras manufactured before summer 2019, including those used in Spinei et al. (2018), was affected by HCHO outgassing from Delrin parts in the sensor head, which made HCHO TCDs from direct-sun measurements unusable in hot environments ( $>28^\circ\text{C}$ ) (Spinei et al., 2020). This issue was resolved by changing the hardware after summer of 2019. The Pandoras used in this research have been manufactured

after summer 2019 and are therefore not affected.

In this paper, all Pandora data were processed with the Blick software version 1.8 (Cede, 2021) and retrieval version nvs3, nvh3, fus5 and fuh5 for total  $\text{NO}_2$ , tropospheric  $\text{NO}_2$ , total HCHO, and tropospheric HCHO VCD, respectively. The detailed description of the retrieval codes can be found in the PGN data product readme ([https://www.pandonia-global-network.org/wp-content/uploads/2023/11/PGN\\_DataProduct\\_s\\_Readme\\_v1-8-8.pdf](https://www.pandonia-global-network.org/wp-content/uploads/2023/11/PGN_DataProduct_s_Readme_v1-8-8.pdf), last access: 2024.07.22). Additionally to fus5 for P189, we used a corrected HCHO TCD data set labeled fus7, where the background polynomial used in the spectral fitting was modified from 4th to 2nd order. In this research, we only use good (0, 10) and medium (1, 11) quality flags for all Pandora products.

### 3.3. GEMS

GEMS is a hyperspectral UV–visible imaging spectrometer that covers the spectral range of 200 to 500 nm with 0.6 nm spectral resolution. GEMS is onboard the GK2B (GEO-KOMPSAT 2B) satellite alongside GOCI-2 (Geostationary Ocean Color Imager-2), launched in February 2020.

Since its launch, GEMS has been continuously monitoring the air

quality over the Asian region (5S-45°N, 75E-145°E) with 3.5 km × 8 km spatial resolution (over Seoul) and an hourly (~ eight times per a day) temporal resolution (Kim et al., 2020). It provides information on vertical columns of NO<sub>2</sub>, O<sub>3</sub>, HCHO, and aerosols with original resolution. For the weak absorbers such as SO<sub>2</sub> and CHOCHO, pixels are co-added to increase the signal-to-noise ratio.

The retrieval of NO<sub>2</sub> is performed with the DOAS fitting algorithm within a 432–450 nm fitting window (Park et al., 2020), while HCHO is derived using the non-linearized fitting method of Basic Optical Absorption Spectroscopy (BOAS) (Chance et al., 2000) in a 329.3–358.6 nm fitting window (Kwon et al., 2019; Lee et al., 2024). In the BOAS method, dSCDs are directly determined by fitting the measured radiance using the nonlinear least squares inversion. The quality of the GEMS retrieval is assessed through flags, which are based on different criteria for each product. The NO<sub>2</sub> product employs a 3-bit binary structure, where each bit represents the good sample or not (0: use, 1: not use), a secondary summary quality flag (0: good, 1: have issue), and bad (not recommended for use). For HCHO, the quality of the retrieval is classified into seven categories: good (0), suspect (1), bad (2), good and suspect of gap-filled pixels (3, 4), missing (−1), and no-data (−999). Detailed description about the quality flags can be found in the GEMS User Guide (<https://nesc.nier.go.kr/en/html/satellite/guide/guide.do>, last access: 2025.01.16). It is recommended to use data with a final algorithm flag of 0 to ensure high accuracy.

In this research, GEMS operational v2.0 total column NO<sub>2</sub> and HCHO products (<https://nesc.nier.go.kr/en/html/datasvc/index.do>, last access: 24 December 2023) are validated. Only pixels with a cloud fraction of <0.33 and a final algorithm flag of 0 were used for evaluation. Additionally, to eliminate persistent outliers in the GEMS HCHO products, we removed unrealistic low (< −2 × 10<sup>16</sup> molec. cm<sup>−2</sup>) and large (> 2 × 10<sup>17</sup> molec. cm<sup>−2</sup>) values. Such extreme values deviate significantly from the range observed by ground-based instruments over the Korean Peninsula (−4 × 10<sup>15</sup> to 7 × 10<sup>16</sup> molec. cm<sup>−2</sup>).

### 3.4. TROPOMI

TROPOMI is a nadir-viewing grating UV-VIS-NIR-SWIR spectrometer (UV: 270–320 nm, VIS: 310–500 nm, NIR: 675–775 nm, SWIR: 2305–2385 nm), onboard the Sentinel-5 Precursor satellite (Veefkind et al., 2012). TROPOMI was launched in October 2017 by ESA to support air quality and climate change research by monitoring gaseous pollutants such as CO, HCHO, CH<sub>4</sub>, NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub>, and aerosols. TROPOMI is passing over Korea ranged from 12:28–14:40 LST and its spatial resolution is 3.5 km × 5.5 km at nadir-view.

The TROPOMI total column (TCD) NO<sub>2</sub> operational product is retrieved from the DOAS spectral fitting method within a 405–465 nm range spectral window by the Royal Netherlands Meteorological Institute (KNMI) (van Geffen et al., 2022).

The HCHO product is also retrieved using DOAS fitting in the spectral window 328.5–359 nm. It uses daily updated reference spectra determined as mean spectra taken over the equatorial Pacific area a day before the measurement. The detailed description of the HCHO retrieval algorithm can be found in De Smedt et al. (2018).

In this research, we use RPRO and OFFL data processed with the v02.04 processor. The bad-quality pixels are removed with the recommended qa<sub>value</sub> of under 0.75 for NO<sub>2</sub> (Eskes and Eichmann, 2023) and under 0.5 for HCHO (De Smedt et al., 2023). Additionally, we removed cloudy pixels with cloud\_fraction\_crb above 0.33 for both NO<sub>2</sub> and HCHO.

## 4. Comparison of Pandora and MAX-DOAS measurements

MAX-DOAS and Pandora instruments are commonly used for the validation of satellite data products (Dimitropoulou et al., 2020; Liu et al., 2023; Peters et al., 2012; Tzortziou et al., 2012; Pinardi et al., 2020., Verhoelst et al., 2021). However, as Pandora retrieves trace gases

with the PGN algorithm, and the MAX-DOAS data used in this work were processed with the MMF algorithm as implemented in the FRM<sub>4</sub>DOAS framework, there is a lack of comparative results between the L2 products retrieved by each class of instruments. This chapter conducts a comparative analysis of NO<sub>2</sub> and HCHO products retrieved using the MMF algorithm applied to IUP-Bremen MAX-DOAS data and the PGN processor applied to Pandora (P189). Both instruments were simultaneously operated on the rooftop of the National Institute of Environmental Research – Environmental Satellite Center (NIER-ESC) in Incheon from July 2022 to November 2022.

The viewing azimuth angles (hereafter, VAA) of MAX-DOAS and Pandora are illustrated in Fig. 1(c). The MAX-DOAS instrument performed sky elevation scans in 5 different VAAs (137.5°, 170°, 185°, 266.5°, and 340°), while the Pandora performed a combination of direct-sun and sky measurements at 300° VAA. To evaluate the effects of aligning the observational geometries of Pandora and MAX-DOAS, the comparison of tropospheric column products was conducted for 3 cases: (1) using MAX-DOAS data from all VAAs, (2) using MAX-DOAS data at 266.5° and 340° VAA, and (3) using the average values between 266.5° and 340° VAA (hereafter, 2-VAA averaged). A coincident measurement data set was created by averaging Pandora data within a 3 min window based on the MAX-DOAS scan time. The 2-VAA averaged MAX-DOAS value was calculated when the difference of observation times between measurements with VAA 266.5° and 340° was <15 min.

We calculate the slope and intercept parameters using a Reduced Major Axis (RMA) regression (Clarke, 1980), as well as mean difference (MD), mean relative difference (MRD), standard deviation, and correlation coefficient. MD is defined as the mean value of the difference between Pandora and MAX-DOAS (Eq. 1) and MRD is a normalized value of MD with MAX-DOAS (Eq. 2). These statistics are also used in section 5 by replacing  $VCD_{Pandora}$  with  $VCD_{GEMS}$  and  $VCD_{MAX-DOAS}$  with  $VCD_{Ground}$

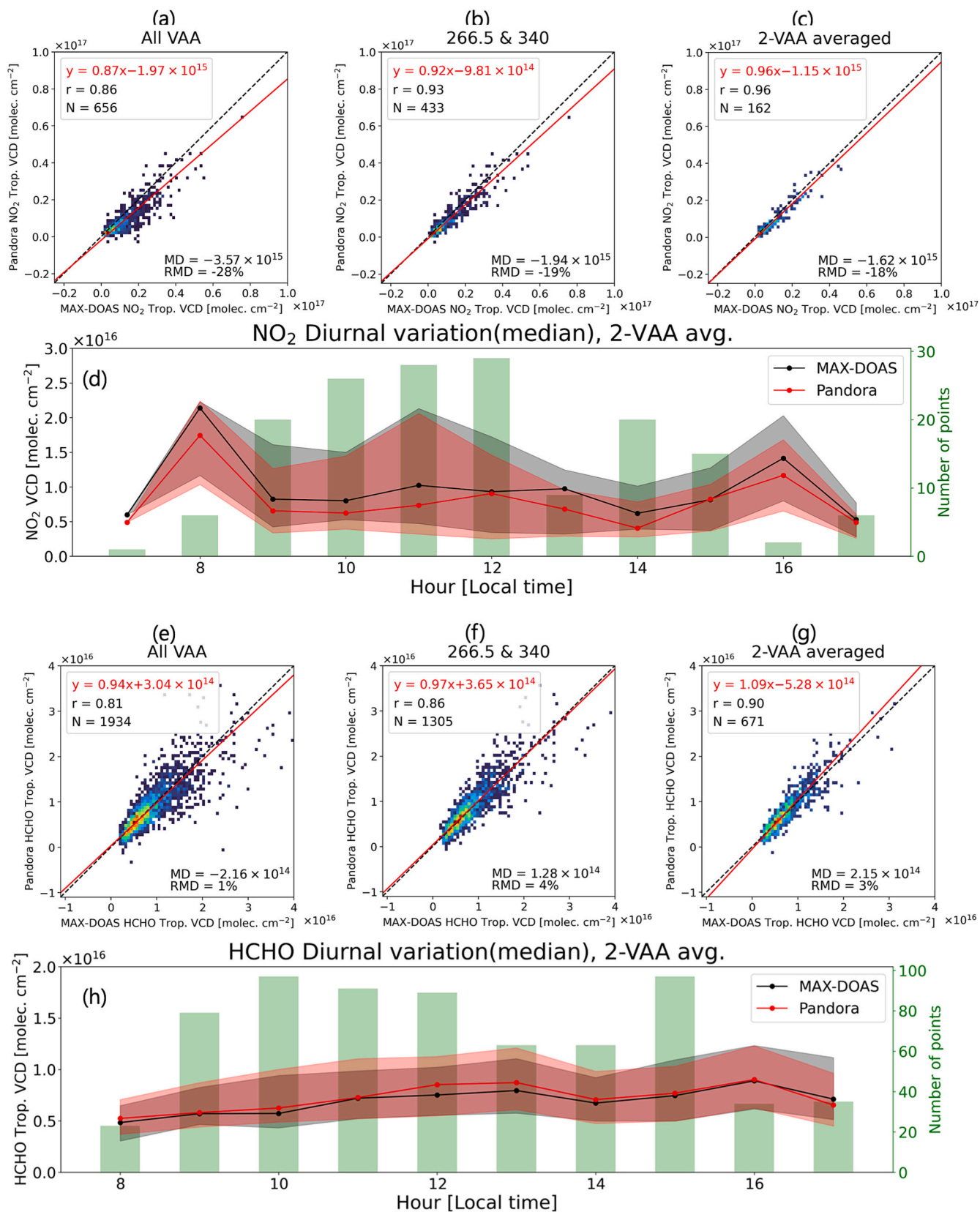
$$MD = \frac{1}{N} \sum_{i=1}^N (VCD_{Pandora,i} - VCD_{MAX-DOAS,i}) \quad (1)$$

$$MRD = \frac{1}{N} \sum_{i=1}^N \left( \frac{VCD_{Pandora,i} - VCD_{MAX-DOAS,i}}{VCD_{MAX-DOAS,i}} \right) \times 100\% \quad (2)$$

### 4.1. Pandora sky measurement vs MAX-DOAS

Comparison results from the different data sets described above are displayed in Fig. 2. Fig. 2(a) compares the tropospheric NO<sub>2</sub> VCDs from Pandora sky measurements at 300° VAA and IUP-Bremen MAX-DOAS data across all VAAs. We find a correlation coefficient of 0.86, however Pandora tropospheric NO<sub>2</sub> columns are lower than the MAX-DOAS columns with a slope of 0.87, a MD of −3.57 × 10<sup>15</sup> molec. cm<sup>−2</sup>, and a MRD of −28 %. The observed discrepancies might be due to the spatial inhomogeneity of NO<sub>2</sub> near the NIER-ESC site as shown in Fig. 1(c): the northwest region of the station, which coincides with the direction of Pandora sky measurements, shows lower NO<sub>2</sub> levels in average compared to the southeast. Consequently, during coincident observation period, the MAX-DOAS instrument observing at VAAs of 137.5°, 170°, and 185° is likely to measure higher VCDs than the Pandora instrument observing at 300° VAA. This interpretation is confirmed when considering MAX-DOAS data acquired at 266.5° and 340° VAA only, as shown in Fig. 2(b). As can be seen, the agreement is significantly improved with a slope of 0.92, a correlation coefficient of 0.93, a MD of −1.94 × 10<sup>15</sup> molec. cm<sup>−2</sup>, and a MRD of −19 %. Furthermore, Fig. 2(c), which compares the MAX-DOAS values averaged from 266.5° and 340°, demonstrates an even better agreement with a slope of 0.96, a correlation coefficient of 0.96, a MD of −1.62 × 10<sup>15</sup> molec. cm<sup>−2</sup>, and a MRD of −18 %.

Although aligning the VAA of both instruments improves the comparison results, Pandora results still show slightly lower tropospheric NO<sub>2</sub> VCDs than the MAX-DOAS columns. This discrepancy may



**Fig. 2.** Comparison of Pandora and MAX-DOAS tropospheric NO<sub>2</sub> VCD (panels a-d) and tropospheric HCHO VCD (panels e-h) in Incheon from July 2022 to November 2022. Panels (a) to (c) are scatter density plots between Pandora (y-axis) and MAX-DOAS (x-axis) of (a) all VAA, (b) 266.5° and 340°, and (c) 2-VAA averaged. Panel (d) is the diurnal variation of tropospheric NO<sub>2</sub> columns observed from 2-VAA averaged MAX-DOAS (black) and Pandora (red). The solid line depicts the median value, top and bottom of the shade are 25 and 75 percentiles of each instrument, and the green bar represents the number of coincident measurement points at each bin. Panels (e)-(h) are the same as (a)-(d), for tropospheric VCD of HCHO.

originate from algorithmic differences such as assumptions on aerosols, the a priori profile of  $\text{NO}_2$ , and the radiative transfer calculation. The MMF algorithm directly runs radiative transfer simulations by utilizing the VLIDORT (Spurr, 2006) model which allows for explicit treatment of light interactions with aerosols and trace gases. In contrast, the PGN algorithm employs a simplified approach where tropospheric vertical columns and profiles are derived from a set of simplified equations making use of  $\text{O}_4$  dSCDs measured at a limited number of elevation angles (see Frieß et al., 2019, and the PGN documentation available online). The PGN algorithm uses spectra observed at elevation angles of  $15^\circ$ ,  $30^\circ$ , and  $90^\circ$  (Cede and Tiefengraber, 2023) while the MMF processes spectra from more elevation angles ( $1^\circ$ ,  $2^\circ$ ,  $3^\circ$ ,  $4^\circ$ ,  $5^\circ$ ,  $6^\circ$ ,  $8^\circ$ ,  $15^\circ$ ,  $30^\circ$ , and  $90^\circ$ ). The inclusion of lower elevation angles enhances the sensitivity close to the surface. Although Pandora data show slightly lower tropospheric  $\text{NO}_2$  columns, both instruments observe consistent diurnal variations, with double peaks at 8 and 16 LST, which correspond to rush hours.

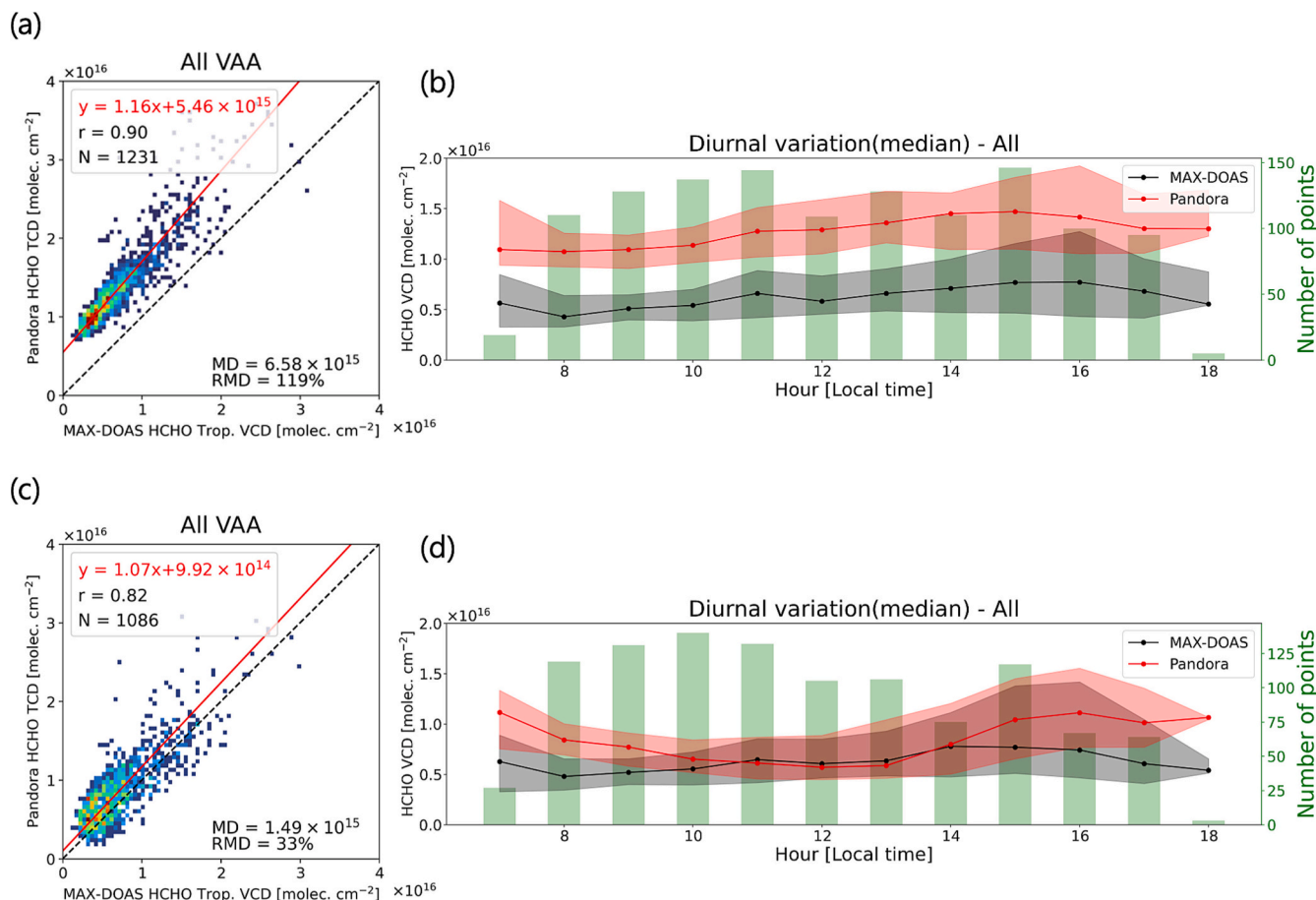
The tropospheric HCHO VCD retrieved from Pandora sky measurements is currently distributed as an unvalidated product. Here, we compare it to the IUP-Bremen MAX-DOAS data to assess its accuracy and suitability for use as a reference for GEMS validation. Like for tropospheric  $\text{NO}_2$ , panels (e) and (g) from Fig. 2 show that aligning the VAA of MAX-DOAS and Pandora instruments also leads to a better agreement between the HCHO measurements. However, in comparison to  $\text{NO}_2$ , the alignment of the viewing geometry had a smaller impact on the agreement between Pandora and MAX-DOAS HCHO measurements. The slope

changes from 0.94 to 1.09, and the correlation coefficient increases from 0.81 to 0.90. This suggests that while HCHO also exhibits spatial inhomogeneity, the magnitude is less pronounced than for  $\text{NO}_2$ . The diurnal pattern of HCHO in Incheon generally exhibits a monotonic increase throughout the day, with slight decreases observed around 14 and 17 LST. This pattern can be attributed to two key factors. First, HCHO is primarily formed through atmospheric photochemical reactions, which are enhanced by rising temperatures and solar shortwave radiation, leading to its typical behavior of having minimum levels in the early morning, increasing throughout the afternoon, and decreasing in the evening again. Second, the direct emissions from mobile sources can explain the increasing HCHO concentration. Considering the diurnal pattern of  $\text{NO}_2$ , high traffic volumes around 16 LST in Incheon likely contribute to the continued increase in HCHO levels, rather than a decrease. This pattern is similarly observed by both instruments.

The agreement found between Pandora and MAX-DOAS HCHO measurements is similar to the one obtained in previous studies comparing different MAX-DOAS instruments (Kreher et al., 2020; Pinardi et al., 2013; Tirpitz et al., 2021).

#### 4.2. Pandora direct-sun measurement vs MAX-DOAS

Fig. 3(a) presents a comparison between the HCHO total columns (TCD) from Pandora direct-sun measurements and tropospheric HCHO VCD from the IUP-Bremen MAX-DOAS instrument. A good correlation is found between the two data sets with a correlation coefficient of 0.90,



**Fig. 3.** Comparison results for Pandora direct-sun products (HCHO TCD) and MAX-DOAS (HCHO tropospheric VCD) in Incheon from July 2022 to November 2022. Panel (a) is a comparison of result between Pandora HCHO TCD and MAX-DOAS tropospheric HCHO VCD. Panel (b) shows the diurnal variation of the median column of MAX-DOAS (black) and Pandora (red). The top and bottom of the shade represent the 25th and 75th percentile of each instrument and the green bar is the number of coincident points. Panel (c) and (d) are the same as (a) and (b), but with a different Pandora retrieval, using a 2nd order background polynomial in the spectral fitting.

however the Pandora HCHO TCDs are substantially larger compared to the MAX-DOAS tropospheric VCD HCHO with a slope of 1.16, a MD of  $6.58 \times 10^{15}$  molec.  $\text{cm}^{-2}$  and a MRD of 119 %. The MAX-DOAS measured the tropospheric HCHO VCD and Pandora direct-sun measurement provided HCHO total column, so it is expected that Pandora direct-sun data are larger than the simultaneous MAX-DOAS data. We examined data from the GEOS-Chem model and from the KORUS-AQ (Korea U.S.-Air Quality) field campaign (Herman et al., 2018) that reported HCHO vertical profiles up to 8 km measured by the Compact Atmospheric Multispecies Spectrometer (CAMS) (Richter et al., 2015), as well as HCHO profiles up to 5 km obtained from the DC-8 aircraft (Kwon et al., 2021). All these data show that the HCHO column above 4 km is small in comparison to the observed discrepancy between the Pandora direct-sun and MAX-DOAS observations. After consultation with the PGN team, a revised direct-sun data set was provided for P189. This version has a slightly modified spectral retrieval scheme where a 2nd order polynomial closure parameter is used instead of the usual 4th order one. This change was made because the instrumental spectral feature was biasing the 4th order background polynomial leading to a cross-correlation with the HCHO retrieval. By changing to a 2nd order polynomial, this bias was removed, but at the cost of a higher uncertainty. As a result of this change (see Figs. 3(c) and (d)) the MD decreased from  $6.58 \times 10^{15}$  molec.  $\text{cm}^{-2}$  to  $1.49 \times 10^{15}$  molec.  $\text{cm}^{-2}$  and the MRD from 119 % to 33 %. We note however that the change in retrieval settings also leads to an increase of the reported mean uncertainty from  $9.83 \times 10^{14}$  molec.  $\text{cm}^{-2}$  to  $2.36 \times 10^{15}$  molec.  $\text{cm}^{-2}$  (see Fig. A.3). In terms of the diurnal variation, shown in Fig. 3(d), the MAX-DOAS and the corrected Pandora data set show different diurnal patterns. The bias correction was most significant between 10 and 14 LST; thus, the corrected Pandora HCHO TCD shows U-shaped pattern with a local minimum at 13 LST, while the MAX-DOAS HCHO VCD shows a monotonic increase from 9 LST to 14 LST. Notably, in Fig. A.3 (b), the reported total uncertainty significantly increased between 10 and 15 LST, the period when the bias correction was most effective.

## 5. GEMS NO<sub>2</sub> and HCHO validation

### 5.1. Total column NO<sub>2</sub>

In this section, we only focus on the evaluation of NO<sub>2</sub> TCDs from operational v2.0 algorithm. Note that Lange et al. (2024) evaluated the GEMS tropospheric NO<sub>2</sub> VCD product using the same MAX-DOAS stations as listed in Table 1.

For total column NO<sub>2</sub> validation, only GEMS pixels that contain the Pandora station are used to optimize the spatial coincidence between satellite and reference data. Pandora data are averaged within a  $\pm 30$  min window centered around the satellite scan time. Both GEMS and Pandora data are filtered with quality criteria as described in Section 3.

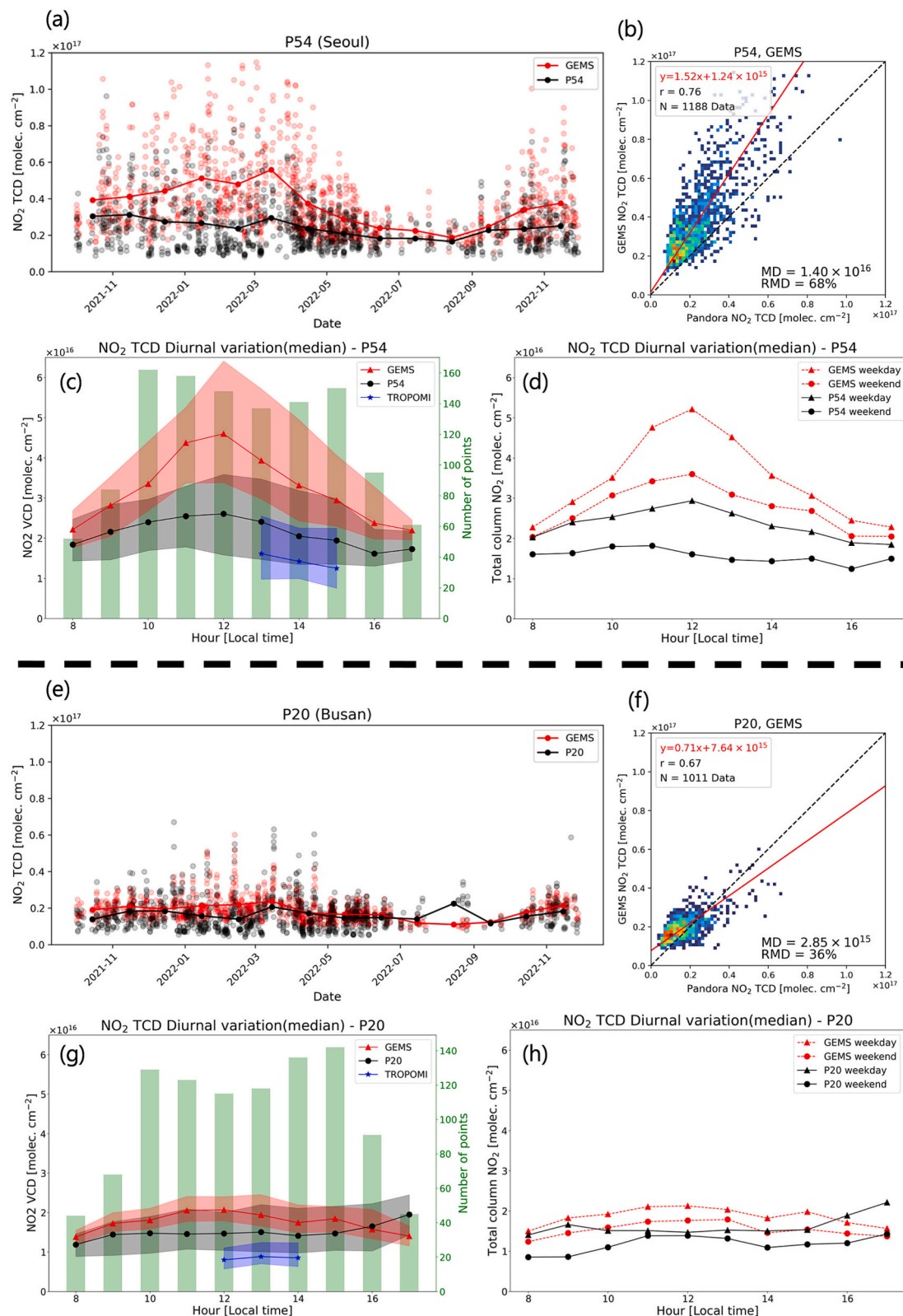
Fig. 4 presents the comparison of GEMS total column NO<sub>2</sub> at station P54 (Seoul) and P20 (Busan). The statistics for all Pandora stations in Korea are summarized in table A.1. Due to its larger urban scale and high anthropogenic NO<sub>x</sub> emissions, Seoul generally shows higher NO<sub>2</sub> TCDs compared to Busan. GEMS captures well the typical seasonal cycle with higher values in winter and lower values in the summer season (Choi et al., 2021; Jang et al., 2017). Similar to the previous GEMS NO<sub>2</sub> VCD validation research by Kim et al. (2023), Edwards et al. (2024), and Lange et al. (2024), the statistical analysis indicates that GEMS overestimates the NO<sub>2</sub> VCD compared to both Pandora instruments (P54 and P20), with MD of  $1.40 \times 10^{16}$  molec.  $\text{cm}^{-2}$  and  $2.85 \times 10^{15}$  molec.  $\text{cm}^{-2}$ , and MRD of 68 % and 36 %, respectively. This overestimation is higher in winter. Notably, at P20, the Product Evaluation of GEMS L2 via Assessment with S5P and Other Sensors (PEGASOS) report (Eichmann et al., personal communication, 2024) also shows consistent results. However, for P20, there was a larger number of instances where GEMS observed smaller TCD than the Pandora instrument, with differences larger than  $1 \times 10^{15}$  molec.  $\text{cm}^{-2}$ . Nevertheless, in terms of correlation,

GEMS and Pandora instruments (P54 and P20) show fair agreement with correlation coefficient of 0.76 and 0.65, respectively. Fig. A.4 shows the validation results of both GEMS and TROPOMI at coincident measurement times. In both stations, GEMS tends to also overestimate TROPOMI.

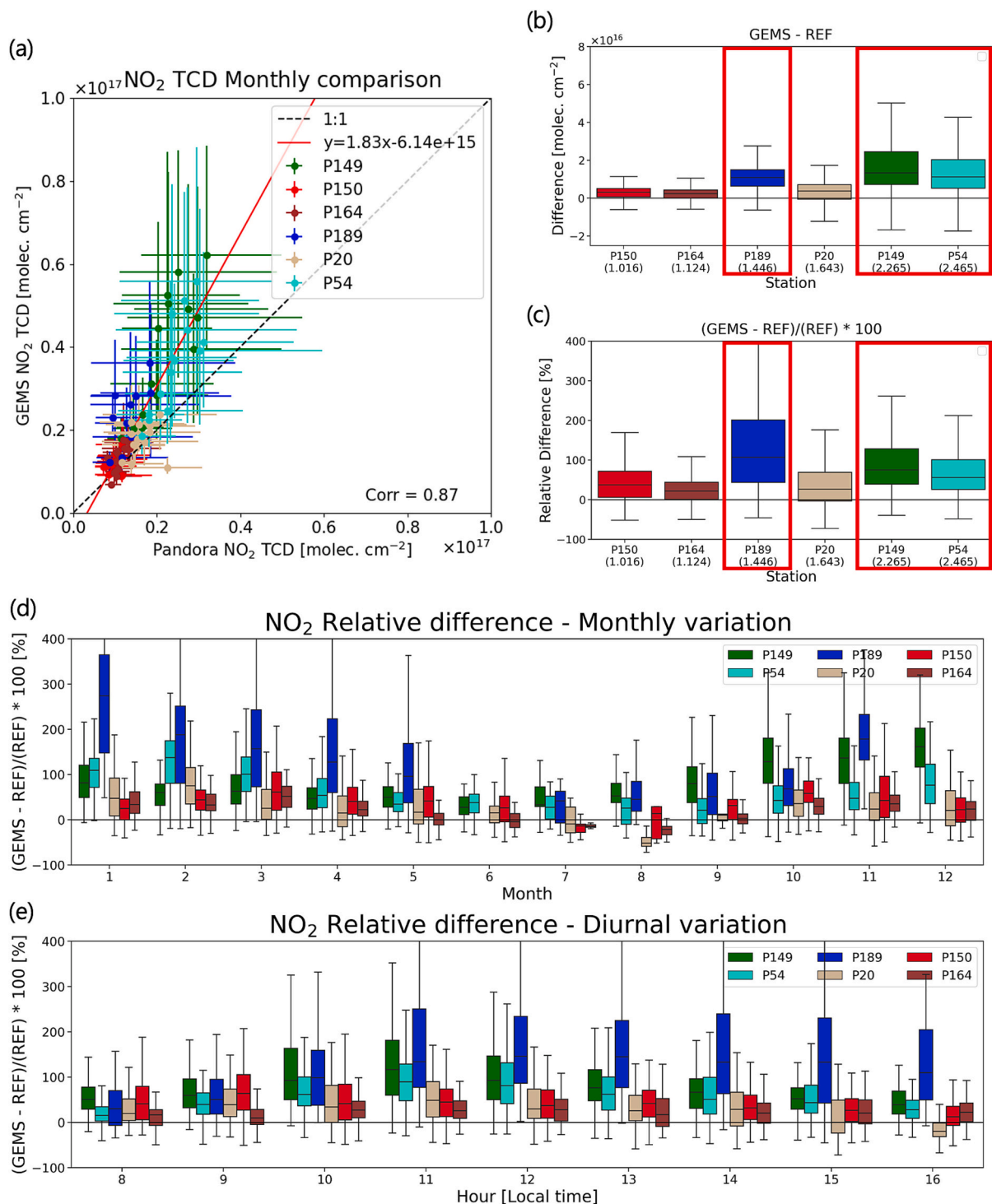
Fig. 4(d) and (h) shows the diurnal variation of NO<sub>2</sub> TCDs at P54 and P20 separated into weekdays and weekend. At P54 (Seoul), both Pandora and GEMS observe the same diurnal pattern during weekdays with an increase in the morning, a peak at noon, and a decrease in the afternoon. GEMS shows higher NO<sub>2</sub> TCDs compared to Pandora during the entire period, but the magnitude of the overestimation is significantly higher around noon. Furthermore, both show higher columns on weekdays. The difference between GEMS and Pandora VCDs is significantly larger during weekdays than during weekends. Additionally, as seen in Fig. 4(a), discrepancies between GEMS and P54 are smaller in summer but become more pronounced in winter and early spring. Since winter and early spring contribute a larger number of comparisons than summer, their influence on the diurnal variability shown in Fig. 4(c) and (d) is greater. This suggests that the seasonal bias is also reflected in the diurnal variation plots.

At the P20 site, the diurnal patterns of NO<sub>2</sub> TCDs observed by GEMS and Pandora differ. The diurnal pattern of the NO<sub>2</sub> TCD observed by GEMS at the P20 site is similar to the diurnal pattern observed by GEMS at the location of P54, exhibiting an inverted U shape with a peak at noontime, whereas the Pandora showed fairly constant NO<sub>2</sub> VCDs until 14 LST and an increase afterwards. The weekend/weekday analysis (see Fig. 4(h)) reveals that both Pandora and GEMS observe similar diurnal patterns on weekends, but differ on weekdays: Pandora observes a U-shaped pattern with the lowest value at noontime while GEMS observes a similar pattern as during weekends, leading to a discrepancy in diurnal patterns between GEMS and Pandora. We cannot conclude the exact cause of the discrepancy in diurnal patterns between GEMS and Pandora in Busan with the current observational data. However, NO<sub>2</sub> spatial inhomogeneity is suggested as a potential contributing factor. Judd et al. (2019) analyzed the impact of spatial resolution on comparisons between satellite data and Pandora using Geostationary Trace gas and Aerosol Sensor Optimization (GeoTASO) airborne measurements collected from May to June 2017 over the western shore of Lake Michigan and the Los Angeles Basin. Their results showed that the coarse spatial resolution of OMI (18 km  $\times$  18 km) was insufficient to capture the fine-scale spatial features within urban areas compared to the higher resolution of TROPOMI (5 km  $\times$  5 km). This study focused on large urban centers in the United States, smaller cities like Busan may require observation with even higher spatial resolution to address these challenges. Lange et al. (2024) investigated the diurnal pattern discrepancy between GEMS and Pandora in Busan by analyzing high-wind ( $\geq 3$  m/s) and low-wind ( $< 3$  m/s) conditions separately. They found that under windy conditions, the Pandora captured an increase in NO<sub>2</sub> VCD during the late afternoon, whereas GEMS did not. This discrepancy may be attributed to local transport. This finding suggests that NO<sub>2</sub> hotspots occurring at spatial scales smaller than the satellite resolution can lead to discrepancies between satellite retrievals and Pandora observations. For observations at larger SZAs, AMFs are expected to be more uncertain. This uncertainty is further enhanced for larger aerosol loads and with low boundary layer heights in the morning and evening. Investigations are planned to explore this issue in more detail.

The validation results for all Pandora stations over Korea from October 2021 to November 2022 are shown in Fig. 5. Overall, the GEMS NO<sub>2</sub> TCD product tends to be larger than the Pandora observations over Korea, with a slope of 1.83, a correlation coefficient of 0.87, an MD of  $7.39 \times 10^{15}$  molec.  $\text{cm}^{-2}$ , and an MRD of 41 %. The SMA region (P189, P149, P54, indicated with red boxes in Fig. 5(b) and (c)) exhibits a larger magnitude of overestimation with an MD of  $1.35 \times 10^{16}$  molec.  $\text{cm}^{-2}$  and an MRD of 67 %, while non-SMA region stations (P20, P150, P164) show an MD of  $1.85 \times 10^{15}$  molec.  $\text{cm}^{-2}$  and an MRD of 17 %. The box-



**Fig. 4.** Comparison of hourly GEMS total column NO<sub>2</sub> for P54 (panels a-d) and P20 (panels e-h). Black, red, and blue color indicate Pandora, GEMS, and TROPOMI data, respectively. Panel (a) and (e) are the timeseries of Pandora and GEMS observations. Transparent dots are hourly data and solid lines with solid dots represent the monthly averaged data. Panel (b) and (f) show the scatter density plot between Pandora (x-axis) and GEMS (y-axis) with RMA regression (red solid line). Panel (c) and (g) are the diurnal variation during the entire period. The shaded region covers the 25 to 75 percentiles of each instrument, and the gray bars represents the number of points at each hour (right hand axes). Panels (d) and (h) are diurnal variations of weekday (triangle) and weekend (circle) of GEMS (red) and Pandora (black).



**Fig. 5.** Overall validation results of GEMS total column  $\text{NO}_2$ . (a) Scatter plot of monthly averaged total column  $\text{NO}_2$  of GEMS and Pandora with error bars from 10th to 90th percentile. Box-whisker plot of (b) MD and (c) MRD. Stations are sorted by the mean value of Pandora as indicated below the station number in units of  $10^{16} \text{ molec. cm}^{-2}$  and the red boxes represent the SMA region instruments. Panel (d) and (e) are the box-whisker plot of monthly and diurnal variation of the MRD.

whisker plots of MRD in Fig. 5(d) and (e) demonstrate seasonal and diurnal variations of the MRD. The MRD shows the minimum in summer, and the maximum in winter, decreasing from March to August, which is followed by an increase. The MRD shows an additional diurnal variation, with a maximum around noon and being lowest in the morning and evening. It should be noted that this diurnal variation of MRD includes one year of data. Early morning and late afternoon data are mainly from the summer season, whereas data around noon represent all seasons (see Fig. A.2). Consequently, the observed diurnal

pattern of MRD reflects a combination of real diurnal bias variation and bias variation caused by seasonal dependencies. Such overestimations can be mitigated through improvements in the AMF calculations. Lange et al. (2024) compared the GEMS operational  $\text{NO}_2$  product with the scientific product retrieved by the IUP Bremen. The key differences regarding the AMF are the use of actual daily TM5  $\text{NO}_2$  vertical profile shapes, the replacement of the GEMS surface reflectivity product with TROPOMI Lambertian Equivalent Reflectivity (LER), and the use of SCIATRAN (Rozanov et al., 2014) instead of VLIDORT for radiative

transfer calculations. The overestimation was smaller in the scientific product compared to the operational product. The GEMS NO<sub>2</sub> IUP Bremen scientific product using the GEMS surface reflectivity product instead of the TROPOMI LER product, exhibits a larger bias compared to the scientific product retrieved using the TROPOMI LER.

## 5.2. Total column HCHO

The current operational GEMS HCHO v2.0 algorithm only provides the HCHO total columns. However, the bulk of HCHO is in the lower troposphere and to keep the continuity with previous studies by Kwon et al. (2019) and Lee et al. (2024), the tropospheric HCHO VCD obtained from both MAX-DOAS and sky measurements of Pandora instruments are used.

Due to the higher retrieval noise of HCHO compared to NO<sub>2</sub>, we use the average value of the GEMS pixels withing a 10 km radius from each station for the validation of HCHO. Analogous to the NO<sub>2</sub> analysis, ground-based data are averaged within a  $\pm 30$  min window centered around the satellite scan time. TROPOMI tropospheric HCHO VCDs are also processed with the same method as used for the NO<sub>2</sub> validation.

Fig. 6 illustrates the validation results of the hourly GEMS HCHO product and the ground-based remote sensing instruments at UB Incheon (MAX-DOAS; Incheon), and P150 (Pandora; Ulsan). In Fig. 6(a) and 6(e), GEMS effectively captures the typical seasonal variation of HCHO, with lower values in winter and higher values in summer, resulting from the enhancement of the VOCs oxidation and the increase in biogenic emissions driven by elevated temperature and solar short-wave radiation. The hourly comparison of GEMS with MAX-DOAS data at Incheon and with Pandora data at Ulsan (see Figs. 6(b) and 6(f) respectively), shows different results. Incheon MAX-DOAS data show a good agreement with GEMS with a slope of 0.83 and a correlation coefficient of 0.60, while P150 at Ulsan shows a slope of 0.59 and a correlation coefficient of 0.58. GEMS tends to underestimate high TCDs above  $1 \times 10^{16}$  molec. cm<sup>-2</sup>, a behavior similar to the one observed with NO<sub>2</sub>, and this occurs more frequently in Ulsan than in Incheon. If we overlap TROPOMI and GEMS validation results and only consider GEMS data at the TROPOMI overpass time (Fig. A.5), TROPOMI shows slightly lower correlation coefficients than GEMS but a higher regression slope.

In terms of diurnal variations, GEMS and ground-based instruments show similar patterns at each observation site with small differences in detail. In Incheon, Fig. 6(c), both GEMS and MAX-DOAS report a diurnal pattern of HCHO that remains flat until 15 LST, followed by an increase. However, GEMS shows lower values than MAX-DOAS before noontime. In Fig. 6(g), both GEMS and Pandora in Ulsan capture a similar diurnal pattern of decreasing HCHO VCDs in the morning followed by an increase in the afternoon. However, during 11 to 15 LST, while Pandora gradually increases, GEMS shows a parabolic increase with a local maximum at 13 LST. This discrepancy mainly originates from the autumn (SON) season, as can be seen in Fig. 6(h). As to the seasonal analysis, Incheon shows no significant seasonal difference in its diurnal pattern, only exhibiting HCHO TCDs that are lower in winter and higher in summer. In contrast, Ulsan shows notable differences in its diurnal variation patterns across seasons. In winter and autumn, the diurnal variation as measured by P150 is flat during the day, however GEMS data show an early afternoon peak, especially during autumn. In spring, the HCHO TCD, as measured by GEMS and P150, gradually increases throughout the day. In summer, both GEMS and Pandora exhibit a much steeper increase in VCD until 13 LST compared to other seasons. While Pandora maintains its peak VCD until 16 LST, GEMS shows a slight decrease after 13 LST and then a second peak at 16 LST. Since the P150 station is surrounded by mountains, the biogenic emission may cause this different diurnal pattern in the summer season. One potential reason for the differences in the detailed diurnal patterns observed between GEMS and ground-based remote sensing instruments could be related to background correction. The GEMS HCHO VCD is calculated by adding the background vertical column (VCD<sub>0</sub>) from the CTM to the differential

VCD (dVCD) retrieved from the observed radiance. According to Lee et al. (2024), the contribution of VCD<sub>0</sub> to the final VCD is approximately 70 % higher in GEMS compared to TROPOMI over Northeast Asia, including the Korean Peninsula. This indicates that the GEMS HCHO product relies more heavily on a priori data than TROPOMI. By managing the background correction issue in future updates, it is expected that GEMS will provide more accurate observations of the diurnal pattern of HCHO.

Fig. 7 shows the overall validation results from all MAX-DOAS and Pandora stations during the GMAP/SIJAQ campaign period. As reported by Lee et al. (2024), the correlation between the monthly averages of GEMS and both MAX-DOAS and Pandora data is good, with a correlation coefficient of 0.86 (for both) and a slope of 0.84 and 0.79 respectively. The MD and MRD compared with Pandora instruments were calculated as  $-5.35 \times 10^{14}$  molec. cm<sup>-2</sup> ( $-1.32 \times 10^{15}$  molec. cm<sup>-2</sup> to  $8.02 \times 10^{14}$  molec. cm<sup>-2</sup>) and 18 % ( $-8$  % to 59 %), respectively. Similarly, for all MAX-DOAS instruments, MD and MRD values were  $-2.57 \times 10^{15}$  molec. cm<sup>-2</sup> ( $-4.52 \times 10^{15}$  molec. cm<sup>-2</sup> to  $-1.05 \times 10^{15}$  molec. cm<sup>-2</sup>) and  $-16$  % ( $-40$  % to 5 %). Considering the different MAX-DOAS instruments (see red box in Fig. 7(a)), validation results at BIRA and MPIC stations show significant negative difference suggesting that these instruments tend to report larger HCHO TCD than others. The larger negative bias observed at BIRA (Seoul and Suwon) and MPIC (Olympic) stations is attributed to instrumental and/or ground-based data retrieval issues rather than to GEMS-specific issues at these sites. A similar conclusion was reported in Van Roozendaal et al. (2024). More work is needed to better understand the origin of these apparent discrepancies. Unlike for NO<sub>2</sub> validation results, there is no significant seasonal or diurnal variability in the MD and MRD for HCHO.

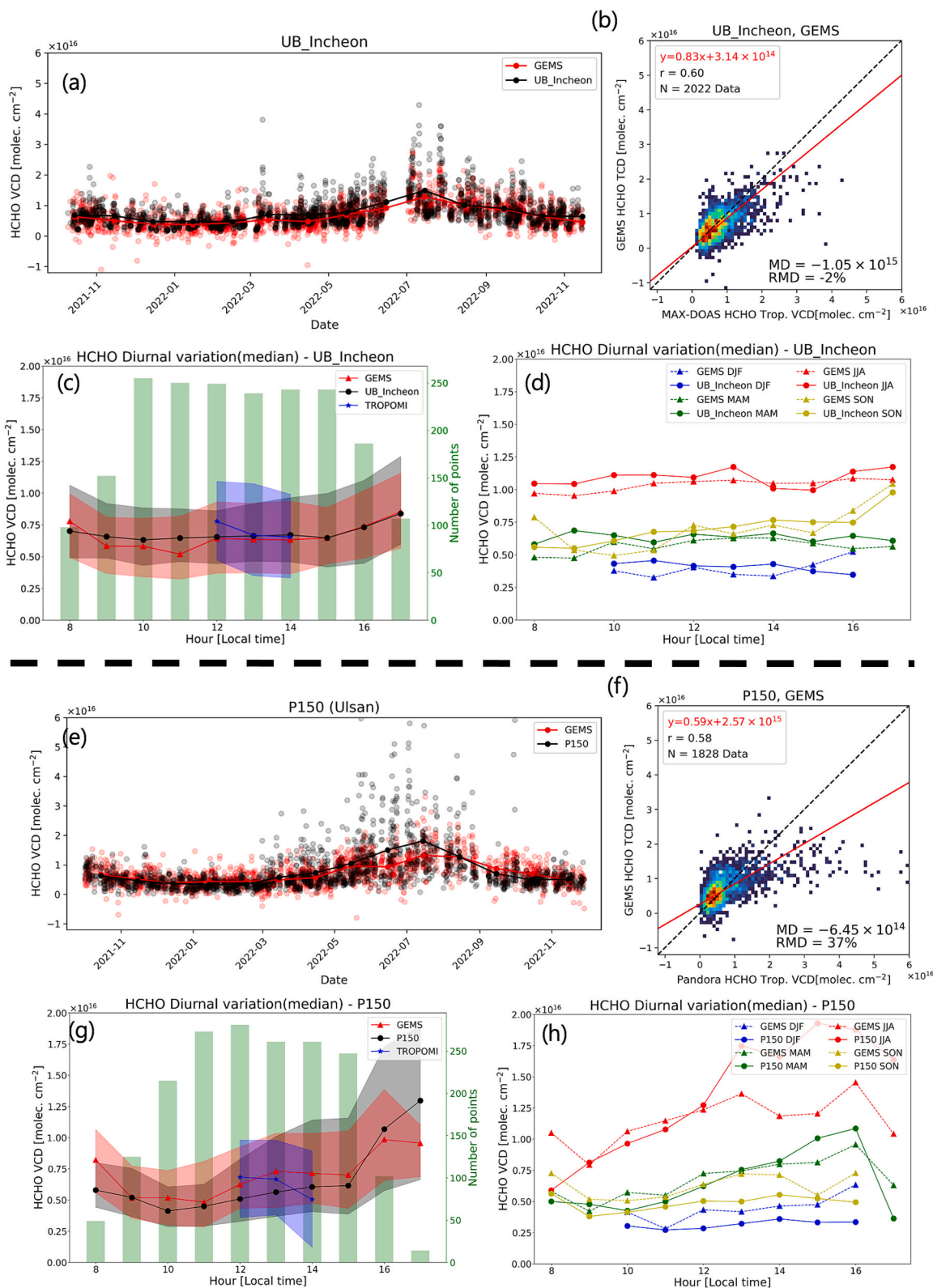
## 6. Conclusion

A comparison between MAX-DOAS and Pandora instruments in Incheon followed by a validation exercise of GEMS operational v2.0 NO<sub>2</sub> and HCHO total column products was conducted during the period October 2021 to November 2022, making use of the data from the GMAP and SIJAQ campaign data sets.

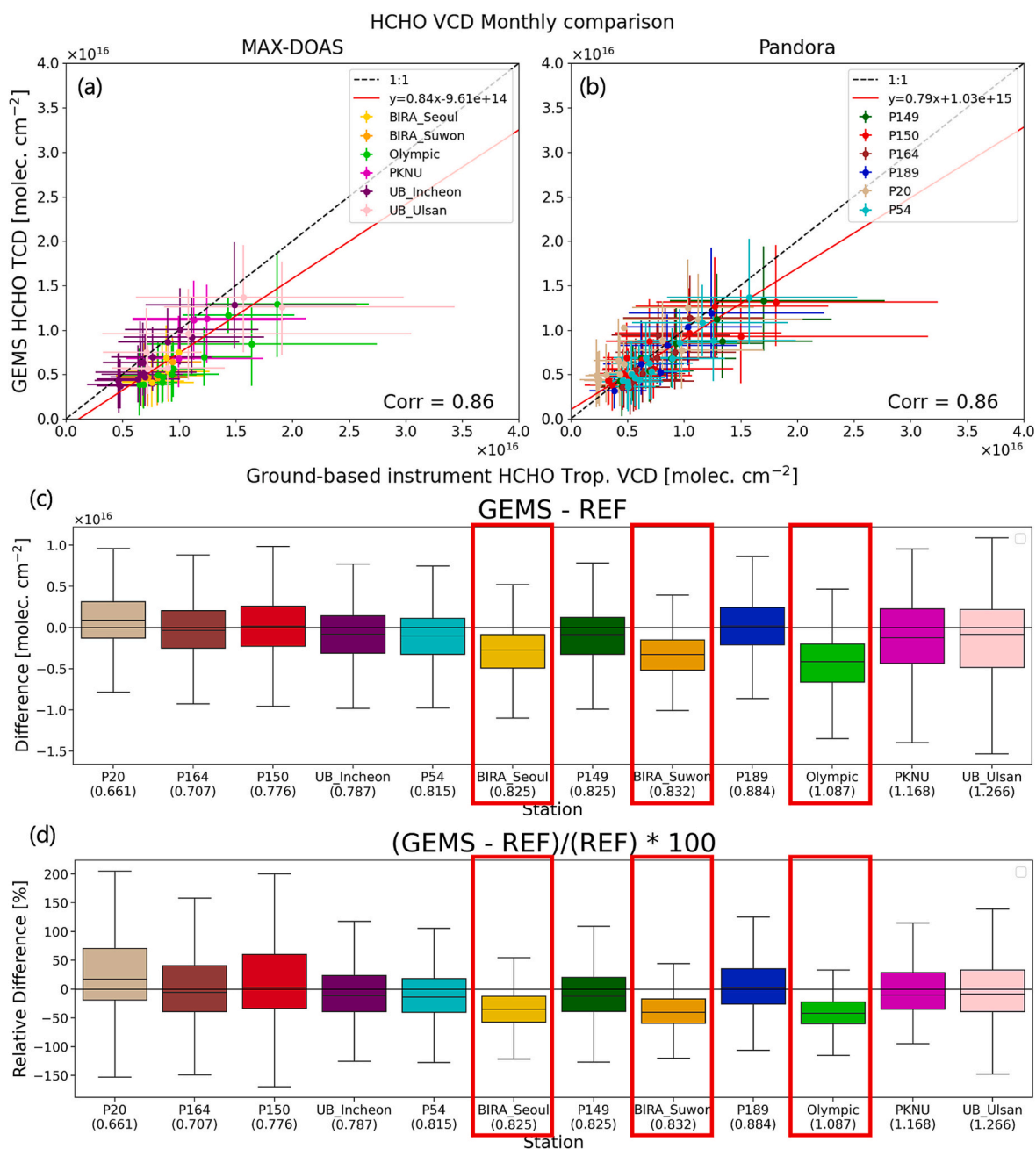
The comparison of tropospheric NO<sub>2</sub> and HCHO VCD between MAX-DOAS and the sky measurements from Pandora shows the importance of aligning the instruments viewing directions. Under aligned conditions, tropospheric NO<sub>2</sub> and HCHO VCDs retrieved from MAX-DOAS and Pandora instruments show good agreement. After proper matching of the viewing geometries, the slope and correlation coefficient increase from 0.87 to 0.96 and 0.86 to 0.96 for tropospheric NO<sub>2</sub> VCD. Similarly, the tropospheric HCHO VCD comparison shows a change in slope from 0.941 to 1.093, and an improvement in the correlation coefficient from 0.81 to 0.90.

The comparison of HCHO total columns from Pandora direct-sun measurements with HCHO tropospheric columns from MAX-DOAS measurements shows a significant discrepancy with a mean difference of  $7.06 \times 10^{15}$  molec. cm<sup>-2</sup> and a relative mean difference ((Pandora-MAX-DOAS)/MAX-DOAS  $\times 100$  %) of 126 %. Revised data provided by the PGN team, using slightly modified retrieval settings, significantly reduces the bias compared to MAX-DOAS results. This correction led to an improvement of the MD and MRD from  $7.06 \times 10^{15}$  molec. cm<sup>-2</sup> to  $1.49 \times 10^{15}$  molec. cm<sup>-2</sup> and 126 % to 33 % respectively. However, this change is also accompanied by an increase of the reported uncertainty from  $9.83 \times 10^{14}$  molec. cm<sup>-2</sup> to  $2.35 \times 10^{15}$  molec. cm<sup>-2</sup>.

Pandora total column NO<sub>2</sub> products from 6 official PGN instruments over Korea were used for validation of GEMS operational v2.0 total column NO<sub>2</sub>. Overall, GEMS shows a good agreement with the station, with a correlation coefficient of 0.87. However, GEMS tends to overestimate Pandora data, showing a slope of 1.83, and a mean relative difference of 41 %. Particularly the SMA region (P54, P149, P189) shows a large overestimation with a MRD of 67 % from GEMS compared to the other stations (P20, P150, P164). The magnitude of the overestimation



**Fig. 6.** Comparison of hourly HCHO TCD from GEMS and HCHO tropospheric VCD from ground-based remote sensing instruments at UB\_Incheon (panels a-d) and P150 (panels e-h) station. Black, red, and blue color indicate ground-based instruments, GEMS, and TROPOMI data respectively. Panel (a) and (e) are the time series plots of ground-based instruments and GEMS. Transparent dots are hourly data and the solid line with solid dots represent the monthly averaged data. Panel (b) and (f) show the scatter density plot between ground-based instruments (x-axis) and GEMS (y-axis) with RMA regression (red solid line). Panel (c) and (g) show the diurnal variation from October 2021 to November 2022. The shaded regions represent the 25 and 75 percentiles of each instrument, and the gray bar is the number of points at each hour. Panel (d) and (h) are diurnal variations during each season (DJF: blue, MAM: green, JJA: red, SON: yellow), dashed-triangle for GEMS and solid-dots for the ground-based instruments.



**Fig. 7.** Overall validation results of the GEMS HCHO product. The monthly scatter plot of averaged GEMS and MAX-DOAS (a) and Pandora (b) data. The black dashed line is 1:1 and the red solid line is the RMA regression line. Panel (c) and (d) are box-whisker plot of the MD and MRD of each station.

of GEMS is more pronounced in highly polluted conditions (i.e. during winter, and at noontime). Despite the reported overestimation, GEMS and Pandora data show similar diurnal patterns and seasonality. The exact cause of the overestimation remains unclear, further investigations are required to fully understand the underlying factors contributing to this discrepancy.

The validation of GEMS operational v2.0 HCHO total columns was conducted using HCHO data from 6 MAX-DOAS stations and 6 Pandora sky measurement. Overall, GEMS shows a good general agreement with both Pandora and MAX-DOAS data, with slopes of 0.84 and 0.80, respectively, and correlation coefficients of 0.86 in monthly averaged comparisons. Large columns, however, tend to be systematically underestimated. Furthermore, GEMS captures well the seasonal and diurnal variations of HCHO and does not display any significant pattern of MB and NMB.

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.scitotenv.2025.179190>.

#### CRediT authorship contribution statement

**Kangho Bae:** Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Chang-Keun Song:** Writing – review & editing, Supervision, Resources. **Michel Van Roozendaal:** Writing – review & editing, Resources, Investigation, Formal analysis. **Andreas Richter:** Writing – review & editing, Resources, Investigation. **Thomas Wagner:** Writing – review & editing, Resources, Investigation. **Alexis Merlaud:** Writing – review & editing, Investigation, Formal analysis. **Gaia Pinardi:** Writing – review & editing, Formal analysis. **Martina M. Friedrich:** Writing – review & editing, Investigation, Formal analysis,

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### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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### Data availability

GEMS L2 NO<sub>2</sub> and HCHO data can be accessed at <https://nesc.nier.go.kr/en/html/cnnts/91/static/page.do> (National Institute of Environmental Research, NIER, last access: 13 August 2024). The TROPOMI NO<sub>2</sub> and HCHO data available at <https://documentation.dataspace.copernicus.eu/Data/SentinelMissions/Sentinel5P.html> (Copernicus dataspace, last access: 23 September 2024). The Pandora data are available from the PGN data archive (<https://data.pandonia-global-network.org/>), last access: 23 September 2024). The FRM<sub>4</sub>DOAS MAX-DOAS data are available on request.

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