

# Challenges and opportunities offered by geostationary space observations for air quality research and emission monitoring

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41 ABSTRACT: Space-borne remote sensing of atmospheric chemical constituents is crucial for  
42 monitoring and better understanding global and regional air quality. Since the 1990s, the continuous  
43 development of instruments onboard low-Earth orbit (LEO) satellites has led to major advances  
44 in air quality research by providing daily global measurements of atmospheric chemical species.  
45 The next generation of atmospheric composition satellites measures from the geostationary Earth  
46 orbit (GEO) with hourly temporal resolution, allowing the observation of diurnal variations of air  
47 pollutants. The first two instruments of the GEO constellation coordinated by the Committee on  
48 Earth Observation Satellites (CEOS), the Geostationary Environment Monitoring Spectrometer  
49 (GEMS) for Asia and the Tropospheric Emissions: Monitoring Pollution (TEMPO) for North  
50 America, were successfully launched in 2020 and 2023, respectively. The European component,  
51 Sentinel-4, is planned for launch in 2025. This work provides an overview of satellite missions for  
52 atmospheric composition monitoring and the state of the science in air quality research. We cover  
53 recent advances in retrieval algorithms, the modeling of emissions and atmospheric chemistry,  
54 data assimilation, and the application of machine learning based on satellite data. We discuss  
55 the challenges and opportunities in air quality research in the era of GEO satellites, and provide  
56 recommendations on research priorities for the near future.

57 SIGNIFICANCE STATEMENT: Space-borne measurements of the chemical composition of the  
58 atmosphere are crucial for understanding and forecasting air quality. With the next generation  
59 of atmospheric composition satellites measuring from the geostationary Earth orbit, air quality  
60 research has entered a new era. We provide an overview of the constellation of satellites for  
61 atmospheric composition monitoring and review the latest advances in satellite-driven air quality  
62 research. We identify the challenges and opportunities for a better exploitation of the wealth of  
63 satellite data from a geostationary perspective.

64 CAPSULE: The International Space Science Institute International Expert Team has reviewed  
65 recent advances and discussed challenges and opportunities in air quality research in the era of  
66 geostationary atmospheric composition satellites.

## 67 **1. Introduction**

68 Air pollution is one of the leading causes of global premature mortality and economic damages  
69 (Cohen et al. 2017; Dechezleprêtre et al. 2019). Space-borne remote sensing instruments have  
70 played a key role in monitoring atmospheric composition since the 1990s (Burrows et al. 1999;  
71 Bovensmann et al. 1999; Drummond and Mand 1996; Veefkind et al. 2006, 2012; Zoogman et al.  
72 2017; Levelt et al. 2018; Kim et al. 2020, among others). Satellite observations have been used  
73 with sophisticated models to help develop policies to reduce emissions (e.g., Duncan et al. 2016;  
74 Jiang et al. 2018), improve our knowledge about air pollution (e.g., Fu et al. 2007; Silvern et al.  
75 2019; Yang et al. 2023b), and better forecast air quality (e.g., Peuch et al. 2022; Eskes et al. 2024).  
76 Efficient reduction of air pollution often contributes to the reduction of co-emitted greenhouse gases  
77 (GHGs) and towards the mitigation of climate change (West et al. 2013; Miyazaki and Bowman  
78 2023).

79 Efforts have been made to improve the observation of atmospheric composition from space over  
80 the past two decades. The TROPOspheric Monitoring Instrument (TROPOMI; 2017–present;  
81 Veefkind et al. 2012) is the first to provide daily global multi-constituent measurements at a sub-  
82 10 km spatial resolution (Veefkind et al. 2012), which helps to reveal detailed linkages between  
83 human activities and air quality (e.g., Riess et al. 2022; Martínez-Alonso et al. 2023; Zuo et al.  
84 2023). The next generation of atmospheric composition monitoring satellites measures column  
85 abundances of trace gases from the geostationary Earth orbit (GEO). The first two GEO atmospheric

composition satellites, GEMS (Geostationary Environment Monitoring Spectrometer; Kim et al. 2020) for Asia and TEMPO (Tropospheric Emissions: Monitoring of Pollution; Zoogman et al. 2017) for North America, were successfully launched in 2020 and 2023, respectively. The European component, Sentinel-4, is planned for launched in 2025 (Stark et al. 2013). Ongoing LEO missions have been proposed to sustain atmospheric composition observations outside the GEO domains.

The International Space Science Institute (ISSI) offers the platform to facilitate international collaboration on interdisciplinary research in space science. The ISSI International Expert Team 489 (Brasseur and Granier 2020) recently assessed advancements in the use of space-borne instruments to improve air quality characterization and forecasts. We summarize the discussion and conclusions from the ISSI Team 489 Workshop (2023) in this paper to provide an overview of the opportunities and challenges arising in the era of GEO atmospheric composition satellites. The recently launched and scheduled satellite instruments motivate us to review the state of air quality research based on satellite observations. We cover advances in the development of retrieval algorithms, modeling and forecasting of air quality, data assimilation, and machine learning applications. We conclude with recommendations for research priorities for the near future to better exploit GEO satellite atmospheric composition observations.

## 2. Constellation of LEO and GEO atmospheric composition satellites

### *a. Heritage of LEO satellites*

Column concentrations of short-lived air pollutants, including tropospheric ozone ( $O_3$ ), nitrogen dioxide ( $NO_2$ ), sulfur dioxide ( $SO_2$ ), formaldehyde (HCHO), and aerosols, are retrieved in the ultraviolet (UV), visible (Vis), and near-infrared (NIR) spectral bands from nadir-viewing satellite instruments. NASA's Backscatter UV (BUV) instruments were the first satellite missions measuring total ozone columns since the 1970s (Mateer et al. 1971; Heath et al. 1975; Frederick et al. 1986; Bhartia et al. 2013). As shown in Table 1, satellites in low-Earth orbit (LEO) provide a nearly daily global coverage and their spatial resolution has improved over time. Compared to GOME (1995–2011; Burrows et al. 1999), the GOME-2 series (2006–present; Munro et al. 2016) measure at four times higher spatial resolution, and the Ozone Monitoring Instrument (OMI; 2004–present; Veefkind et al. 2006) has a further improved spatial resolution ( $13 \times 24 \text{ km}^2$ ). Measurements made by GOME, GOME-2, SCIAMACHY (2002–2012; Bovensmann et al. 1999), and OMI include

important chemical species for atmospheric chemistry and have greatly advanced our understanding of air quality (e.g., Duncan et al. 2016; Levelt et al. 2018). TROPOMI (2017–present) onboard the Copernicus Sentinel-5 Precursor (Sentinel-5P) mission measures from UV-Vis-NIR to short-wave infrared (SWIR), which allows the measurements of an extended list of trace gases (Veefkind et al. 2012). Its unprecedented resolution of  $3.5 \times 5.5 \text{ km}^2$  and the high signal-to-noise ratio reveal enriched details of air pollution, which has greatly advanced air quality research in recent years (e.g., Fioletov et al. 2020; Stavrakou et al. 2020; Riess et al. 2022).

Infrared (IR) instruments also provide measurements about atmospheric composition. The MOPITT (Measurements Of Pollution In The Troposphere; 1999–present; Drummond et al. 2022; Buchholz et al. 2021) instrument measures carbon monoxide (CO) from the short-wave infrared and thermal infrared (TIR), and was one of the first satellite instruments that tracked global pollution transport. The Infrared Atmospheric Sounding Interferometer (IASI; 2006–present; Clerbaux et al. 2009) instruments were launched on the Metop (Meteorological Operational satellite) series, measuring meteorological variables, air pollutants, and greenhouse gases from the TIR with a 12 km footprint resolution. To date, 33 chemical species have been detected above the IASI instrumental noise level (Clarisse et al. 2011; Franco et al. 2018). As a companion to IASI, a series of TIR instruments have been launched by NASA and NOAA, the Atmospheric Infrared Sounder (AIRS; 2002–present; Lambrigtsen et al. 2004) on Aura, and NOAA’s Cross-track Infrared Sounder (CrIS; 2011–present; Han et al. 2013).

Nadir-viewing LEO satellites provide valuable information on the seasonal and interannual variability of atmospheric composition. Rapid changes in emissions are detected, often in real-time, as demonstrated during the lockdowns in response to the COVID-19 spread (Bauwens et al. 2020; Liu et al. 2020a; Gkatzelis et al. 2021, among others). The LEO satellites provide decades of atmospheric composition measurements since the 1990s, allowing trend analysis at different spatial scales (e.g., Lamsal et al. 2015; Duncan et al. 2016; Stavrakou et al. 2018; Hedelius et al. 2021).

#### *b. GEO satellites for atmospheric chemistry*

Atmospheric composition measurements from GEO satellites greatly expand the global observing system for air quality. They can provide continuous observations during daytime hours (24 hours

TABLE 1. Constellation of nadir-viewing LEO and GEO space-borne atmospheric chemistry monitoring instruments since 2000.<sup>a</sup>

Satellite	Instrument	Operation period	Spectral range	Resolution (km <sup>2</sup> )	Coverage <sup>b</sup>	Covered region
LEO						
ERS-2	GOME	1995–2011	UV-Vis	40×320	3 days	Global
Envisat	SCIAMACHY	2002–2012	UV-Vis-SWIR	30×60	6 days	
Aqua	AIRS	2002–present	TIR	13.5×13.5	0.5 day	
Terra	MOPITT	1999–present	NIR-TIR	22×22	5 days	
Metop	GOME-2	2006–present	UV-Vis	40×80	1.5 days	
	IASI		TIR	12×12 <sup>c</sup>	0.5 day	
Aura	OMI	2004–present	UV-Vis	13×24	1 day <sup>d</sup>	
JPSS <sup>e</sup>	OMPS	2012–present	UV-Vis	10×10 <sup>f</sup>	1 day	
	CrIS		TIR	14×14	0.5 day	
Sentinel-5P	TROPOMI	2017–present	UV-Vis-NIR-SWIR	3.5×5.5 <sup>g</sup>	1 day	
Metop-SG A	IASI-NG	2025	TIR	12×12 <sup>c</sup>	0.5 day	
	Sentinel-5		UV-Vis-NIR-SWIR	7.5×7.5	1 day	
GEO						
GK2B	GEMS	2020–present	UV-Vis	3.5×7.7 at 37.5°N	1 hour	East Asia
Intelsat 40e	TEMPO	2023–present	UV-Vis	2.1×4.5 at 36.5°N	1 hour	North America
MTG-S	Sentinel-4	2025	UV-Vis-NIR	8×8 at 45°N	1 hour	Europe and North Africa
	IRS		TIR	4×4 at nadir	1 hour <sup>h</sup>	Europe and Africa
Himawari <sup>i</sup>	AHI	2015–present	Vis-IR	2×2 at nadir	10 minutes <sup>k</sup>	East Asia, Southeast Asia and Oceania
FengYun-4	AGRI	2016–present	Vis-IR	2×2 at nadir	15 minutes <sup>k</sup>	Asia, Southeast Asia and Oceania
	GIIRS		TIR	12×12 <sup>l</sup> at nadir	1.5 hours <sup>m</sup>	
GOES/	ABI	2017–present	Vis-IR	2×2 at nadir	10 minutes <sup>k</sup>	Western Hemisphere
GeoXO	ACX	2035	UV-Vis	8×4 at nadir	1 hour	North America
	GXS		TIR	4×4 at nadir	30 minutes <sup>n</sup>	Western Hemisphere

<sup>a</sup> Instruments dedicated to measuring GHGs are not considered within the scope of the paper. <sup>b</sup> Time required for global coverage for LEO instruments or coverage of the field of regard for GEO instruments. <sup>c</sup> IASI and IASI-NG have a circular pixel geometry of 12 km diameter. <sup>d</sup> The revisit time of OMI was increased to 2–3 days since 2018 due to the OMI row anomaly (Torres et al. 2018). <sup>e</sup> CrIS and OMPS are currently on the Suomi NPP, NOAA-20 and NOAA-21 satellites. They will also fly on the JPSS-3 and -4 satellites. <sup>f</sup> Pixel size of OMPS mapper on Suomi NPP is 50×50 km<sup>2</sup> but improved to 17×13 km<sup>2</sup> on NOAA-20 and then 10×10 km<sup>2</sup> on NOAA-21. OMPS nadir profiler has 250×250 km<sup>2</sup> resolution. <sup>g</sup> Resolution of TROPOMI at nadir observations was increased from 3.5×7 km<sup>2</sup> to 3.5×5.5 km<sup>2</sup> on 6 August 2019. <sup>h</sup> IRS revisit time is 30 minutes over Europe and 1 hour elsewhere. <sup>i</sup> The Advanced Himawari Imager (AHI) is operational on Himawari-8 and Himawari-9. <sup>j</sup> The Advanced Baseline Imager (ABI) is operational on GOES-16, GOES-17, GOES-18, and GOES-19. <sup>k</sup> ABI and AHI scan the full disk of observational coverage every 10 minutes. AGRI scans the full disk every 15 minutes. All three instruments support regional scans at 5 minutes or higher frequencies. <sup>l</sup> Pixel size is 16×16 km<sup>2</sup> for GIIRS on FengYun-4A and is 12×12 km<sup>2</sup> for GIIRS on FengYun-4B. <sup>m</sup> Time required to scan the field of regard is 2 hours for GIIRS on FengYun-4A and is 1.5 hours for GIIRS on FengYun-4B. <sup>n</sup> GXS scans the full disk of observational coverage every 30 minutes. It can also scan the contiguous United States every 15 minutes or scan mesoscale regions every 5 minutes.

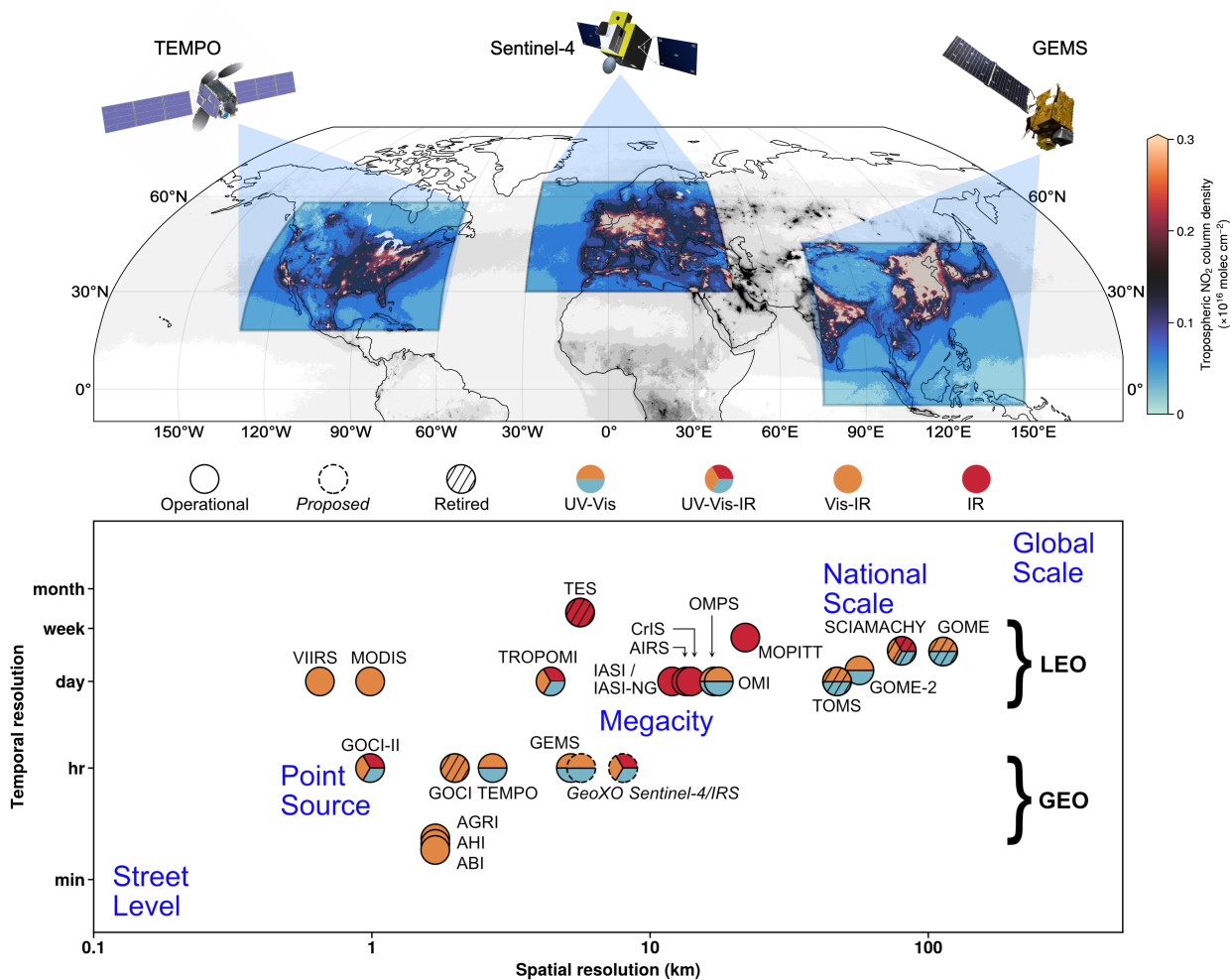


FIG. 1. (Top) Domain and coverage of the GEO satellites. Background is annual mean TROPOMI NO<sub>2</sub> tropospheric columns in 2022. Regions not covered by the GEO satellites are shaded in gray. (Bottom) Spatial and temporal resolution of space-borne instruments for atmospheric composition measurements. Figure adapted from Fig. 1 in Kim et al. (2020).

in the TIR). The geostationary orbit is 36 000 km from the Earth, as compared to ~500 km for LEO, but the weaker photon flux is compensated by a long staring capability so that pixel sizes and precisions from LEO and GEO atmospheric composition instruments are comparable. The same suite of species observable from LEO is also observable from GEO but with much higher data density over the field of regard. The field of regard for a geostationary instrument can be as large as one third of the Earth, although smaller domains are used in the geostationary air quality constellation (see Figure 1) to increase data density and achieve finer pixel resolution.



155 Geostationary satellites observe from fixed longitudes in an equatorial plane, which means that  
156 they have highest resolution at the Equator and limited observation capability for latitudes poleward  
157 of 60 degrees.

158 The Geostationary Interferometric Infrared Sounder (GIIRS) onboard China's FengYun-4 satel-  
159 lite series (FY-4A/B) is the first GEO hyperspectral infrared sounder. FY-4A and FY-4B currently  
160 operate at 86.5°E and 105°E, respectively. The GIIRS observations cover most of East Asia with  
161 a focus on China, with a 2-hour observing cycle. GIIRS measures at a 12 km spatial resolution at  
162 nadir and was recently used to retrieve ammonia (NH<sub>3</sub>; Clarisse et al. 2021; Zeng et al. 2023b),  
163 CO (Zeng et al. 2023a), and formic acid (HCOOH; Zeng et al. 2024). The GIIRS onboard FY-4B  
164 (GIIRS/FY-4B; 2021–present) demonstrates improved sensitivity, better spatial resolution, and  
165 higher accuracy compared to GIIRS/FY-4A (2016–present; Yang et al. 2017). FY-4A/B also carry  
166 the Advanced Geostationary Radiation Imager (AGRI) that measures in Vis and IR.

167 GEMS is the first component of the GEO air quality constellation (see Fig. 1) and measures  
168 aerosols, O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, HCHO, and glyoxal (CHOCHO), over Asia. It measures in UV-Vis with  
169 a spectral resolution of 0.6 nm and a spatial resolution of 3.5 km (NS) × 7.7 km (EW) at Seoul. It  
170 operates above 128.2°E, covering a field of regard from east of Japan to western India (75–145°E)  
171 and from Mongolia to Indonesia (45°N–5°S). GEMS is the first satellite observing the diurnal  
172 variation of air pollution in Asia, including urban pollution, power plants, industrial activities,  
173 ship emissions, wildfires, Asian dust, and volcanic eruptions. Figure 2A shows tropospheric NO<sub>2</sub>  
174 columns measured by GEMS for July 2023. Asian megacities are observed as pollution hot spots.  
175 The diurnal column variations of tropospheric NO<sub>2</sub> columns in Seoul, Beijing and New Delhi show  
176 large disparities due to regional differences in emissions, chemistry, and transport (see Figure 2C).

177 NASA's first Earth Venture Instrument (EVI), TEMPO is hosted onboard the Intelsat-40e satellite  
178 operating above 91°W. Compared to GEMS, TEMPO has a similar spectral resolution and an  
179 additional Vis-NIR channel to enhance retrieval sensitivity for tropospheric O<sub>3</sub> (Zoogman et al.  
180 2017) and aerosols (Chen et al. 2021a). TEMPO scans North America from east to west hourly  
181 with a spatial resolution of 2.1 km (NS) × 4.75 km (EW) at the center of the field of regard  
182 (see Figure 2). TEMPO started its nominal operation in October 2023. The Beta version of data  
183 products was released on NASA's Atmospheric Science Data Center (ASDC) in May 2024 (see  
184 Table 2). Figure 2 shows TEMPO tropospheric NO<sub>2</sub> columns with marked pollution hot spots

185 including the Northeast Corridor, the Canadian oil sands, and the Los Angeles Basin. The observed  
186 diurnal variations of tropospheric NO<sub>2</sub> in New York City and Los Angeles for 17–24 December  
187 2023 show large regional differences as seen by GEMS (see Figure 2B). TEMPO can also measure  
188 the spectral signatures of nighttime lights and differentiate lighting types (Carr et al. 2017).

### 193 *c. Future missions*

194 The Copernicus Sentinel-4 mission will cover Europe, parts of North Africa and parts of the  
195 Atlantic (see Figure 1) centered at a fixed longitude of 0 degrees, with an hourly measuring  
196 frequency similar to GEMS and TEMPO. The operational products include NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub>, aerosols,  
197 as well as the VOC (Volatile Organic Compound) tracers HCHO and CHOCHO. The first Meteosat  
198 Third Generation Sounder (MTG-S1) satellite, expected to be launched in 2025, will carry a  
199 Sentinel-4 instrument on board as well as the Infra-Red Sounder (IRS) (Coopmann et al. 2023).  
200 The IRS has an observational coverage including the entire Africa and Europe. It will measure  
201 every 30 minutes above Europe, and one hour elsewhere in the field of regard, which could be  
202 useful for species with a strong diurnal variability such as NH<sub>3</sub> (see Clarisse et al. 2023).

203 The Geostationary eXtended Observations (GeoXO) mission, NOAA’s next generation GEO  
204 constellation covering the Western Hemisphere, is scheduled for launch in the early 2030s (Lindsey  
205 et al. 2024). The central GeoXO platform (operating above ~105°W) will carry an atmospheric  
206 composition instrument (ACX) in the UV-Vis, as well as a hyperspectral IR sounder (GXS) for  
207 measurements of CO, NH<sub>3</sub>, isoprene, and other VOCs. GeoXO will also carry an imager on  
208 board, similar to the Geostationary Operational Environmental Satellites-16 (GOES-16) Advanced  
209 Baseline Imager (ABI) currently used in various applications. For example, Zhang et al. (2022)  
210 and O’Dell et al. (2024) estimated surface particulate matter (PM<sub>2.5</sub>) concentrations using aerosol  
211 optical depth measurements from GOES-16 and GOES-17. Watine-Guiou et al. (2023) also showed  
212 the potential of using the GOES constellation to monitor methane point sources.

213 IASI-new generation (IASI-NG, Clerbaux and Crevoisier 2013; Crevoisier et al. 2014) is the  
214 follow-on program for IASI, which will be flown onboard the Metop Second Generation (Metop-  
215 SG) satellites. The first Metop-SG platform is planned to be launched in 2025 to LEO and will also  
216 carry the Copernicus Sentinel-5 mission. IASI-NG will have higher spectral resolution and signal-

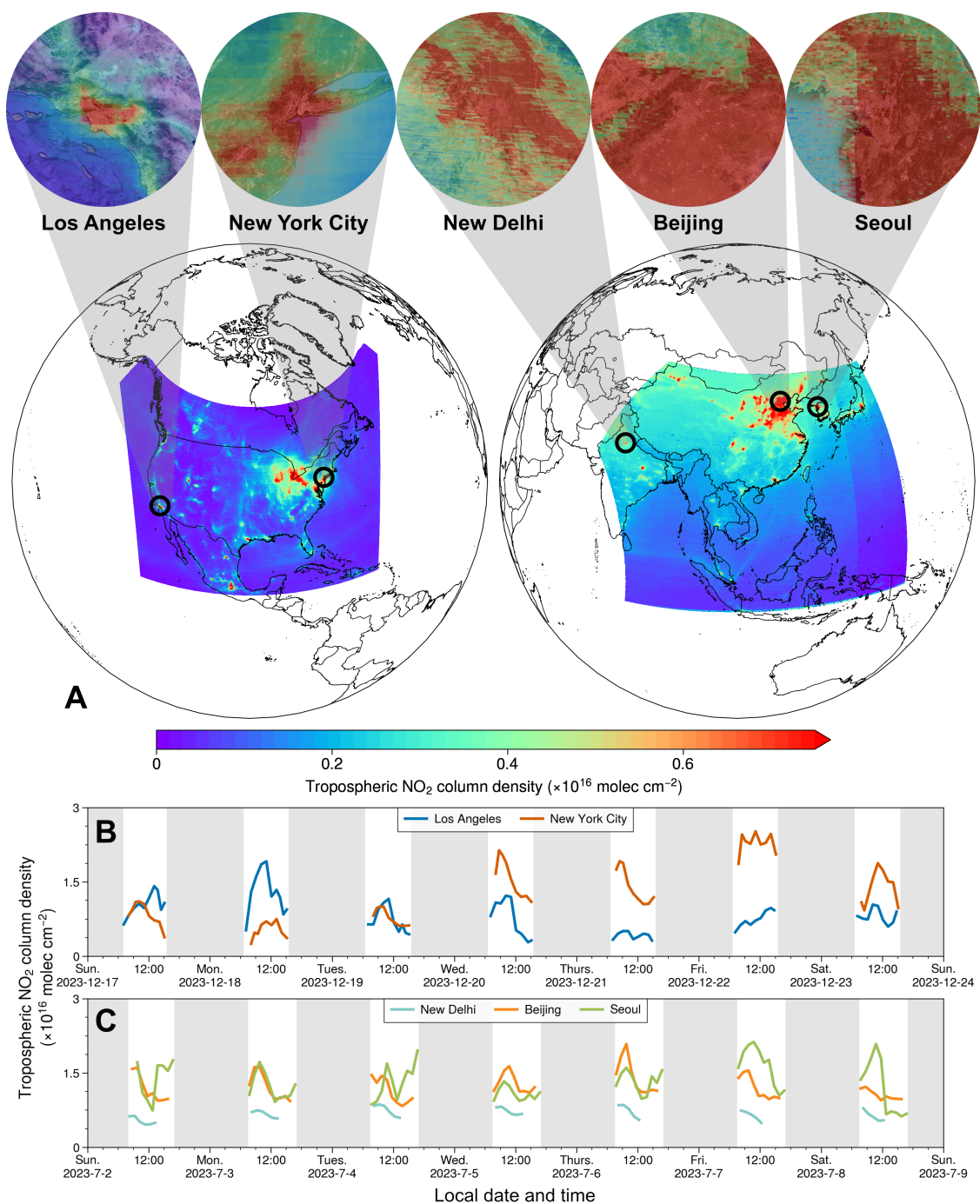


FIG. 2. (A) Illustration of tropospheric  $\text{NO}_2$  column densities measured by TEMPO (left) and GEMS (right). Tropospheric  $\text{NO}_2$  column densities measured over selected cities are shown on top. (B and C) Hourly tropospheric  $\text{NO}_2$  column density measurements show diurnal and weekly cycles over large cities. The TEMPO data set used in this figure is preliminary and unvalidated, and is used for illustration purposes only.

217 to-noise ratio relative to IASI, providing better sensitivity near the surface and an improved vertical  
218 resolution of retrievals. Detection of weak absorbers (e.g.,  $\text{NH}_3$  and  $\text{SO}_2$ ) will also improve.

### 219 **3. Advances in air quality research using space-borne measurements**

220 Over the past few decades, advances in atmospheric composition satellites have set the stage  
221 for air quality research and emission monitoring. The wealth of space observations has driven  
222 progress across all aspects of the research process. In this section, we provide an overview of  
223 recent advances in satellite-based air quality research. In Section 3.a, we review recent progress  
224 in the retrieval of atmospheric composition abundances from satellite measurements. In Sections  
225 3.b and 3.c, we introduce efforts to improve emission estimation and data assimilation techniques,  
226 respectively. Finally, in Section 3.d, we discuss the applications of machine learning in air quality  
227 research.

#### 228 *a. Improved retrieval algorithms*

229 Technological innovations and increasing quality requirements are driving the science of satellite  
230 retrievals forward. For example, significant improvements have been made on retrieval algorithms  
231 for TROPOMI since its launch in 2017, with a focus on better constrained uncertainties and reduced  
232 biases (Theys et al. 2021; Heue et al. 2022; Van Geffen et al. 2022, among others). Besides an  
233 improved degradation correction (Ludewig et al. 2020) and better consistency among retrieval  
234 products (Tilstra et al. 2024), new retrievals from TROPOMI measurements were developed, e.g.,  
235 solar induced fluorescence (SIF; Guanter et al. 2021), aerosol optical depth (Torres et al. 2020),  
236 glyoxal ( $\text{CHOCHO}$ ; Alvarado et al. 2020; Lerot et al. 2021), and nitrous acid ( $\text{HONO}$ ; Theys et al.  
237 2020). An overview of key air pollutants retrieved from space measurements is shown in Table 2.

238 The TROPOMI data products are carefully validated and validation reports are released regularly.  
239 As such, TROPOMI has been used as the reference and transfer standard for the development of  
240 GEMS retrieval algorithms. The first evaluation of GEMS retrievals using TROPOMI and ground-  
241 based measurements showed a good consistency (Baek et al. 2023; Kim et al. 2023). GEMS  
242 measurements captured clear seasonal variations over cities, as well as hourly variations that are  
243 also seen in ground-based remotely sensed columns (Lee et al. 2024). The list of GEMS retrievals

TABLE 2. Air pollutants retrieved from operational space-borne instruments, with DOIs to data products or references

Instruments	NO <sub>2</sub>	O <sub>3</sub>	SO <sub>2</sub>	VOC		Aerosols	HONO	CO	NH <sub>3</sub>
LEO									
TROPOMI	10.5270/ SSP-9bnp8q8	10.5270/ SSP-hcp1l2m	10.5270/ SSP-74eiddi	HCHO	10.5270/ SSP-vg1i7t0	10.5270/ SSP-7g4iapn	10.18758/ 71021058	10.5270/ SSP-bj3nry0	Not measured
				CHOCHO	10.18758/ 4oaroxyf				
OMI	10.5067/Aura/ OMI/DATA2018	10.5067/Aura/ OMI/DATA2013	10.5067/Aura/ OMI/DATA2023	HCHO	10.5067/ Aura/OMI/ DATA2015	10.5067/ Aura/OMI/ DATA2001	Not measured		
GOME-2	Available at EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF)								
IASI	Not measured	Available at AERIS atmospheric data center					10.5281/ zenodo. 10721381	Available at AERIS	
OMPS	10.5067/ NOXVLE2QAVR3	10.5067/ 0WF4HAZ0VHK	10.5067/ A9002ZH0194R	HCHO	10.5067/ IIM1GHT07QA8	10.5067/ 40L92G8144IV	Not measured		
CrS	Not measured	10.5067/ WUKWENW76N5P	Hyman and Pavolonis (2020)	HCHO	Fu et al. (2019)	Not measured	10.5067/ BYIIUV3PR9L6	10.5067/ 713KMUCCJNEN	
Other LEO satellites	Not available	TES: 10.5067/ AURA/TES/ TL203N.008	MLS: 10.5067/Aura/ MLS/DATA2519	Not available	VIIRS: 10.5067/ VIIRS/AERDB_ L2_VIIRS_ SNPP.002	Not avail- able	MOPITT: 10.5067/ TERRA/ MOPITT/ MOP03JM.009	AIRS: 10.5067/ EYXLPVGTSWFF	
GEO									
GEMS	Available from National Institute of Environmental Research, Environmental Satellite Center								
TEMPO	10.5067/ IS-40e/TEMPO/ NO2_L2.001	10.5067/ IS-40e/TEMPO/ O3TOT_L2.003	Not available	HCHO	10.5067/ IS-40e/ TEMPO/HCHO_ L2.001	Not available	Not measured		
FY-4A/B (GIIRS)	Not measured		Not available	Available from Fengyun Data Center		Not mea- sured	10.18170/ DVN/M7DKKL	10.18170/DVN/ VJ4MLO	

244 was recently extended to SO<sub>2</sub> (Park and Jeong 2021), aerosols (Cho et al. 2023; Park et al. 2023),  
245 and glyoxal (Ha et al. 2024).

246 Continued efforts to improve retrieval algorithms have led to new data products for older missions  
247 like OMI, e.g., SO<sub>2</sub> (Li et al. 2022) and O<sub>3</sub> (Bak et al. 2024). Thermal infrared measurements are  
248 now better utilized to monitor extreme events, such as wildfires (Vu Van et al. 2023; Luo et al. 2024)  
249 and volcanic activities (Taylor et al. 2018). Notably, the phenomenal 2022 Hunga Tonga–Hunga  
250 Ha’apai eruption was well observed by thermal infrared spectrometers (e.g., Wright et al. 2022).  
251 The IASI NH<sub>3</sub> and ethylene (C<sub>2</sub>H<sub>4</sub>) retrievals were used to identify point sources from industrial  
252 and agricultural sectors (Van Damme et al. 2018; Franco et al. 2022).

253 The signal-to-noise ratio remains a limiting factor for the retrieval of weakly-absorbing trace  
254 gases (e.g., formaldehyde, SO<sub>2</sub>, and NH<sub>3</sub>). Some recent studies average satellite measurements  
255 over longer time periods to obtain a significant signal (e.g., Van Damme et al. 2018). For more  
256 strongly absorbing gases, like NO<sub>2</sub>, sources of retrieval uncertainties include surface reflectivity,  
257 clouds and aerosols, and aspects like thermal contrast for infrared measurements. Atmospheric  
258 profiles have a strong impact on retrievals in the UV-Vis due to the altitude dependency of Rayleigh  
259 scattering, which becomes more important as the spatial resolution increases (Lamsal et al. 2021).  
260 Averaging kernels have been used in the validation of retrievals and data assimilation to account  
261 for the information content of the retrievals (Eskes and Boersma 2003).

262 To use satellite data at a higher spatial resolution, new oversampling methods have been developed  
263 (Valin et al. 2013; Fioletov et al. 2015; Sun et al. 2018; Van Damme et al. 2018; Clarisse et al. 2019,  
264 among others). For retrievals over emission hotspots, the assumptions about the vertical distribution  
265 of gases (averaging kernels and air mass factors) are particularly important for the quantification  
266 of tropospheric amounts and diurnal variations (Yang et al. 2023b). Regional models capable  
267 of achieving 10 km resolution are being used to provide a priori information for high-resolution  
268 retrieval products (e.g., Liu et al. 2020b for NO<sub>2</sub> in Asia, and Douros et al. (2023) for NO<sub>2</sub> in  
269 Europe).

## 270 *b. Estimation of emissions*

271 The development of emission inventories remains challenging due to the large number of species  
272 taken into account, the variety of emission sources, and because the a priori information is typically

collected by networks that are spatially and temporally sparse (Granier et al. 2023; Sindelarova et al. 2023). For instance, the activity data and emission factors for anthropogenic emissions are available from diverse agencies, such as the International Energy Agency, but public access to this information is often limited. The development of open-source databases has been led by intergovernmental organizations, e.g., the Intergovernmental Panel on Climate Change Emissions Factor Database (IPCC EFDB) or the United Nations Framework Convention on Climate Change (UNFCCC), both of which are built on the data released in national reports. Global emission inventories are generally available with a delay of three to four years. To support policy-making and air quality applications, techniques have been developed to extrapolate emissions to the most recent years (Soulie et al. 2023). The development of emission inventories also need to incorporate a finer temporal resolution and detailed categorization by specific emission sectors. To this end, temporal profiles based on statistical information (e.g., traffic counts) and meteorological parametrizations are typically considered (e.g., Guevara et al. 2021). Additional constraints on temporal profiles can be obtained from the hourly GEO observations, especially the diurnal variations of emissions (Park et al. 2024). Table 3 lists the main publicly available emission inventories, covering both pollutants and greenhouse gases at global and regional scales.

Large discrepancies have been highlighted among emission inventories due to differences in the activity data and emission factors (Elguindi et al. 2020; Granier et al. 2023). Complementary to the emission inventories, a growing number of studies (cf. Section 3.c) use satellite observations and inverse modeling techniques to estimate emissions, namely NO<sub>x</sub> (e.g., Stavrakou et al. 2008; Kurokawa et al. 2009; Miyazaki et al. 2017; Jiang et al. 2022; Plauchu et al. 2024; van der A et al. 2024), VOCs (e.g., Millet et al. 2008; Stavrakou et al. 2012; Marais et al. 2012; Bauwens et al. 2016; Cao et al. 2018; Oomen et al. 2024; Müller et al. 2024), CO (e.g., Arellano et al. 2004; Müller et al. 2018; Qu et al. 2022b) and greenhouse gases (e.g., Wang et al. 2018; Lu et al. 2021). Figure 3 illustrates a comparison of NO<sub>x</sub> emissions in China from 2000 to 2020 from several emission inventories and satellite-based emission estimates (Elguindi et al. 2020). The differences between various estimates remain significant, especially for the trends, which underscores the need for continued efforts on mitigating uncertainties in emissions.

The development of new retrievals (see Section 3.a) has advanced emission estimates from both natural and anthropogenic sources. For example, the new TROPOMI HONO retrieval product

TABLE 3. List of several global and regional publicly available emissions inventories

Acronym	Time period covered	Spatial resolution (degree <sup>2</sup> )	Temporal resolution	Species considered	DOI or reference
<b>Global inventory</b>					
EDGARv8	1970–2022	0.1x0.1	Monthly	Pollutants+GHGs	Crippa et al. (2023a, 2024)
HTAPv3	2000–2018	0.1x0.1	Monthly	Pollutants	Crippa et al. (2023b)
CEDS	1980–2019	0.1x0.1	Monthly	Pollutants+GHGs	10.25584/PNNLDH/1854347
CAMS-GLOB-ANT v6.2	2000–2025	0.1x0.1	Monthly	Pollutants+GHGs	10.24380/eets-qd81
ECLIPSE v6	1990–2050 (by 5 or 10 yrs)	0.5x0.5	Yearly	Pollutants+CH <sub>4</sub>	Klimont et al. (2017)
<b>Regional inventory</b>					
CAMS-REG (Europe)	2000–2022	0.1x0.05	Yearly	Pollutants+GHGs	Kuennen et al. (2021)
EMEP (Europe)	1990–2022	No grid	Yearly	Pollutants	European Environment Agency (2023)
EPA <sup>a</sup> (USA)	1970–2023	No grid	Yearly	Pollutants+GHGs	epa.gov
Government Canada	1990–2022	No grid	Yearly	Pollutants+GHGs	Environment and Climate Change Canada (2019); Government of Canada (2018)
PAPIL A (Latin America)	2014–2020	0.1x0.1	Yearly	Pollutants+GHGs	10.5281/zenodo.12944491
DACCIWA (Africa)	1990–2015	0.1x0.1	Yearly	Pollutants	Keita et al. (2021)
MIXv2 (Asia)	2010–2017	0.1x0.1	Monthly	Pollutants+CO <sub>2</sub>	Li et al. 2023b
REASv3.2 (Asia)	1950–2015	0.25x0.25	Monthly	Pollutants+CO <sub>2</sub>	Kurokawa and Ohara (2020)
MEIC 1.4 (China)	1990–2020	0.25x0.25	Monthly	Pollutants+CO <sub>2</sub>	Zheng et al. (2018)

<sup>a</sup> Table shows the EPA Air Pollutant Emissions Trends Data. The EPA National Emissions Inventory (NEI) are available every three years with variable resolutions from 36 km to 4 km.



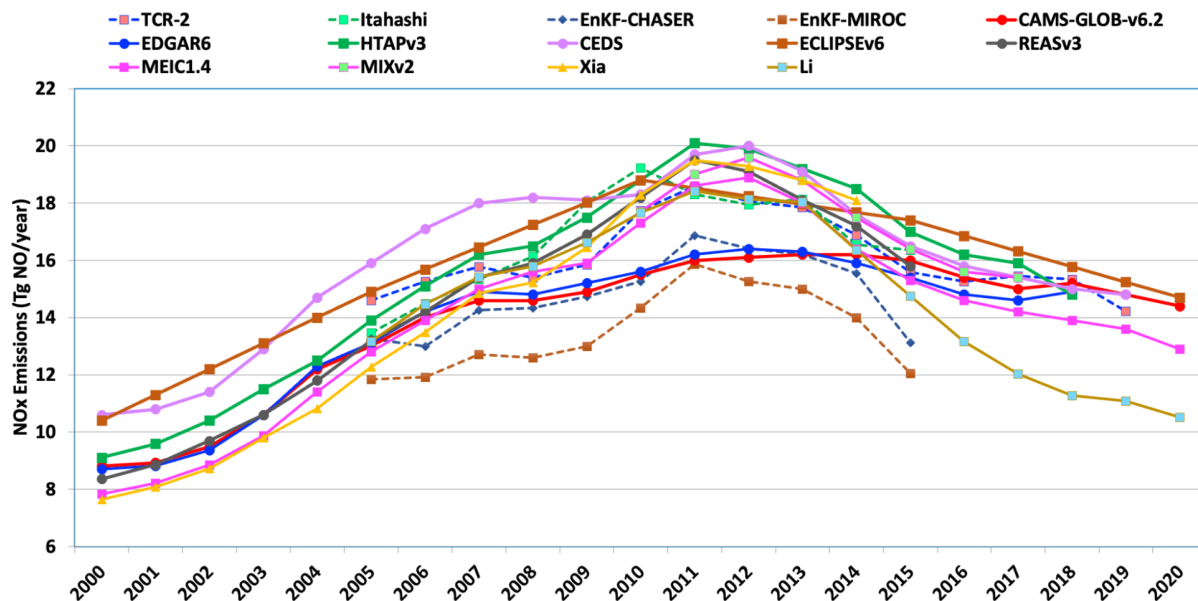


FIG. 3. Comparison of annual mean NO<sub>x</sub> emissions in China from 2000 to 2020 (in Tg NO<sub>x</sub>-NO/yr) from several datasets. Solid and dashed lines represent emission inventories and satellite-based emission estimates, respectively. The references for the emission estimates are shown in the legend on top. Figure adapted from Elguindi et al. (2020).

shows intense emissions in wildfire plumes, accounting for a substantial share of total hydroxyl radical (OH) production from natural sources (Theys et al. 2020). The first global satellite isoprene retrievals from CrIS (Fu et al. 2019), combined with HCHO observations, have been used to constrain isoprene emissions and atmospheric oxidation (Wells et al. 2020). These analyses reveal significantly underestimated isoprene emissions in emission inventories, particularly in tropical regions (Wells et al. 2020). The use of satellite retrievals has also proven to be crucial for identifying seasonalities and weekly patterns in emissions, providing complementary information to temporal profiles derived from activity data. This is particularly valuable for sources with limited activity information, such as those in the agricultural sector (e.g., Damme et al. 2022). Wind rotation method is another important advancement that estimates point source emissions by resolving emission plumes aligned with the wind direction (e.g., Beirle et al. 2011; Valin et al. 2013; Fioletov et al. 2015; Clarisse et al. 2019).

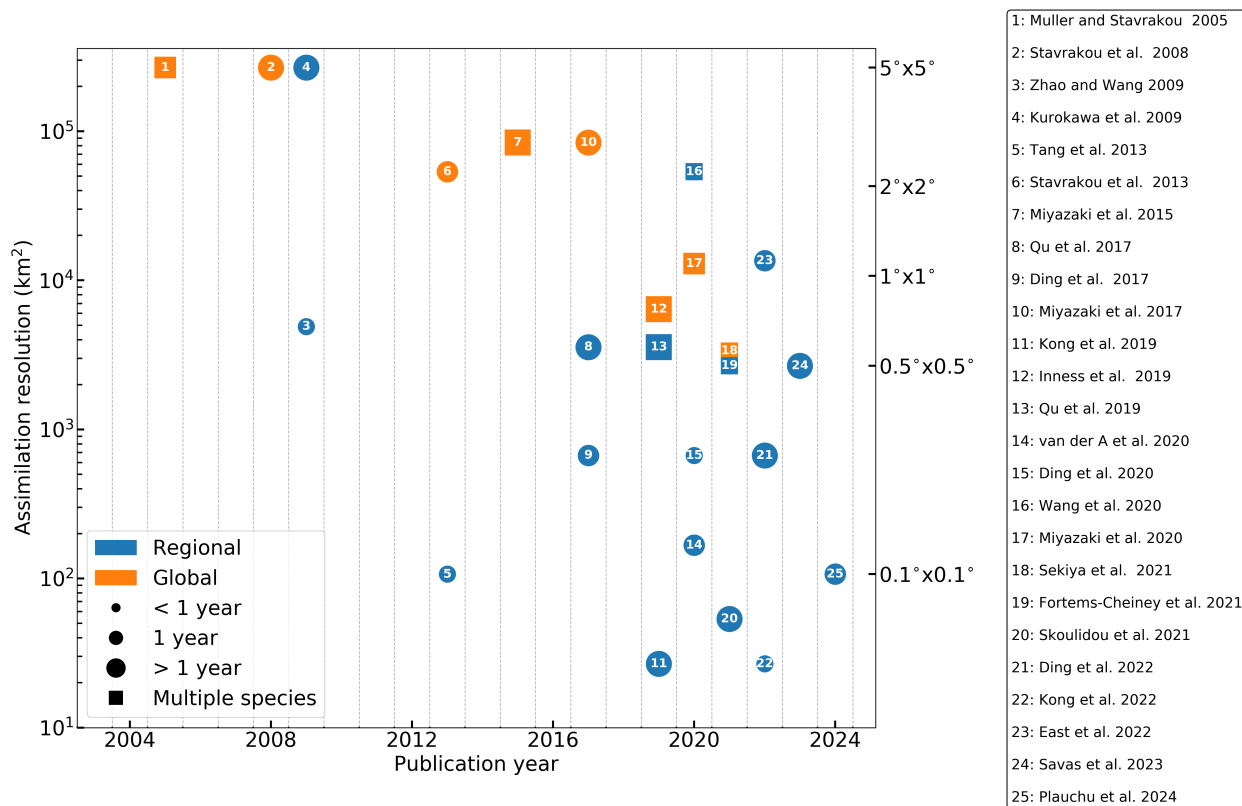


FIG. 4. Evolution of the spatial resolution of space-based NO<sub>2</sub> data assimilation studies over the past two decades. Orange symbols denote global studies, blue symbols denote regional studies. Circles describe data assimilation systems in which only NO<sub>2</sub> is assimilated. Squares represent multi-species data assimilation studies. The size of the symbol represents the temporal scale.

### c. Advances in data assimilation

Data assimilation in air quality research combines observations with chemical transport models (CTMs) to produce an analysis of the state of atmospheric composition (e.g., Carmichael et al. 2008; Lahoz and Schneider 2014). Areas of application include air quality forecasting (e.g., Inness et al. 2015), inverse modeling of emissions and other model parameters, and constructing reanalyses of atmospheric composition. Numerous advances have been achieved in data assimilation in the past decades, owing to improved satellite retrievals, better parameterized models, and advanced assimilation techniques (Sandu and Chai 2011; Streets et al. 2013; Bocquet et al. 2015). For examples shown in Figure 4, the assimilation of space-based NO<sub>2</sub> data has evolved to increasingly high spatial resolution in recent years.

Data assimilation techniques solve for the statistically optimal solution based on observations and models (Kalnay et al. 2007). Filtering approaches such as the ensemble Kalman filter (EnKF) capture chemical non-linearities using an ensemble of models and estimate emissions at regional (Tang et al. 2013; Yumimoto et al. 2014; Gaubert et al. 2020; Feng et al. 2020; Dai et al. 2021; van der Graaf et al. 2022) and global (Miyazaki et al. 2012, 2020a; Gaubert et al. 2023) scales. The 4D-Var method utilizes the adjoint of forward models to minimize the model-observation mismatch. Although the development of adjoint models can be complex and running them can be computationally costly, 4D-Var has been successfully implemented for various applications (Elbern et al. 2000; Müller and Stavrakou 2005; Henze et al. 2007). 4D-Var is also used in the Integrated Forecasting System (IFS) of the European Union's Copernicus Atmosphere Monitoring Service (CAMS) (Inness et al. 2015, 2019, 2022).

Simultaneous joint assimilations of multiple species, such as CO/NO<sub>2</sub> (Müller and Stavrakou 2005), HCHO/CHOCHO (Stavrakou et al. 2009; Cao et al. 2018), SO<sub>2</sub>/NO<sub>2</sub> (Qu et al. 2019; Wang et al. 2020), and NO<sub>2</sub>/CO/SO<sub>2</sub> (Miyazaki et al. 2017, 2020a,b), have shown to improve data assimilation results, as it accounts for the impact of emission changes on the chemical lifetimes of various species. Specifically, assimilating short-lived species can help better characterize the budget of longer-lived gases (e.g., Gaubert et al. 2017; Zheng et al. 2019). To address the increased computational cost of multi-species data assimilation, hybrid approaches combining 3D-Var and mass balance have been recently developed to improve the computational efficiency (Li and Xiao 2019; Chen et al. 2021b).

#### *d. Application of machine learning*

Machine learning has recently become a popular choice for satellite retrievals due to its higher computational efficiency with respect to traditional retrieval methods. One of the first machine learning applications widely used in data products is the operational IASI NH<sub>3</sub> retrievals based on neural networks (Whitburn et al. 2016; Van Damme et al. 2017). Following that, new data products have been developed for IASI, e.g., the acetone and ethylene retrievals (Franco et al. 2019, 2022), and the CrIS data products (Wells et al. 2022, 2024).

An emerging application of machine learning studies is the estimation of surface concentrations using neural networks and tree-based models for PM<sub>2.5</sub> (Di et al. 2019; Wei et al. 2020; Pendergrass

et al. 2022), O<sub>3</sub> (Sayeed et al. 2021; Betancourt et al. 2022), NO<sub>2</sub> (Di et al. 2020; Ghahremanloo et al. 2021; Chan et al. 2021), CO (Han et al. 2022; Chen et al. 2024), and CH<sub>4</sub> (Balasus et al. 2023). These studies rely on the fusion of data from multiple sources and show improved skill compared to conventional approaches (Balasus et al. 2023; Oak et al. 2024; Huang et al. 2024). Other research directions include the development of surrogate models or modules in conventional modeling systems with an improved efficiency (Keller and Evans 2019; Kelp et al. 2020, 2022; He et al. 2024b). Using machine learning to understand drivers of air pollution (Zhang et al. 2023; Ma et al. 2023; Wang et al. 2024) and conduct trend analysis (He et al. 2022a; Pendergrass et al. 2022, 2024; Li et al. 2023a) are other intriguing directions. The potential of machine learning in the inverse modeling of emissions has also been explored (Huang et al. 2021; He et al. 2022b).

#### 4. Challenges and opportunities in the era of geostationary space observations

Space observations from GEO offer a number of opportunities for improved characterization of air quality and emissions as compared to LEO observations. The higher observation density due to more frequent return times allows for higher precision. It also facilitates cloud clearing, meaning an increased probability of observing a cloud-free scene in a certain location (or adjacent locations) over a certain time period. The continuous observation available from GEO instruments enables the tracking of pollution transport on meso- and synoptic scales. Multiple measurements during the day provide information on the diurnal variations of emissions and chemical evolution. However, there are also important challenges in the retrieval and the interpretation of GEO observations. Next, we elaborate on the opportunities and challenges in retrieval development (Section 4.a), atmospheric composition modeling (Section 4.b), data assimilation (Section 4.c), and machine learning applications for GEO observations (Section 4.d), and we discuss air quality research for large world regions that are not covered by the planned GEO satellite constellation (Section 4.e).

##### *a. Retrievals*

For GEO observations, not only do the pollutant concentrations change over the day, but the position of the Sun, the surface temperature, the vertical mixing of the atmosphere, and meteorology also change. These parameters are either input variables or impact the a priori vertical profile of

389 the trace gases being retrieved, of which the hourly variations need to be accounted for in retrieval  
390 algorithms.

391 An important aspect is the variation in surface reflectivity for UV-Vis retrievals. Larger reflec-  
392 tivity increases the sensitivity of satellite measurements to trace gases close to the surface, and  
393 not considering the diurnal variations in surface reflectivity could lead to artifacts in the retrieved  
394 diurnal variation of pollutants. While surface reflectivity information is available from satellite ob-  
395 servations, the temporal and spatial resolution may not be sufficient, and uncertainties can be large  
396 for individual observations. A similar problem exists for TIR retrievals, where surface radiation  
397 emission is strongly dependent on temperature.

398 A second challenge is the diurnal variation due to vertical mixing, which can change the sensitivity  
399 of the satellite measurements to different vertical layers in the atmosphere (Yang et al. 2023a). For  
400 UV-Vis retrievals, sensitivity is usually lowest close to the surface, and a shallow boundary layer in  
401 the morning reduces sensitivity compared to a fully developed boundary layer in the afternoon. The  
402 situation can further be complicated by residual aerosols above the boundary layer. Similar issues  
403 are expected from the combination of vertical trace gas distributions and temperature profiles for  
404 TIR observations. To account for these effects, atmospheric models used as a priori information in  
405 retrievals must reflect the diurnal evolution of the boundary layer, which can be challenging over  
406 complex urban areas and terrain.

407 The viewing geometry from GEO can also present challenges, especially for higher latitudes  
408 and at the edges of the field of regard. For UV-Vis observations, large viewing zenith angles  
409 can lead to increased scattering in the atmosphere and reduced sensitivity to trace gases near the  
410 surface. The effect is further amplified by the presence of aerosols and clouds. In addition, spatial  
411 oversampling is generally of limited use for GEO observations due to the constant ground pixel  
412 pattern, as reported in Lange et al. (2024) for the case of GEMS. A possible solution would be  
413 to adjust the latitudinal pointing and longitudinal sampling of GEO measurements, but this may  
414 complicate the interpretation of the observed diurnal variations and affect the aerosol and cloud  
415 measurements, which depend on accurate surface reflectance characterization.

416 For some trace gases, such as  $O_3$  and  $NO_2$ , significant amounts are present in both the troposphere  
417 and the stratosphere. This necessitates a stratospheric correction, which, in the case of GEO  
418 observations, also needs to account for the diurnal change of the stratospheric amounts. This is

419 particularly relevant for small signals, which are more affected by uncertainties in the stratospheric  
420 correction.

421 Given the challenges outlined above, robust calibration and validation of GEO observations  
422 becomes essential to ensure a consistent retrieval quality across different sensors and GEO regions.  
423 The calibration and validation efforts for GEO observations will build on the experience from  
424 heritage LEO missions (CEOS 2019). These efforts should be supplemented by intensive ground-  
425 based and aircraft validation campaigns to evaluate the diurnal patterns measured by the GEO  
426 satellites (see e.g. Kim et al. 2023; Lee et al. 2024; Lange et al. 2024; Ha et al. 2024). LEO  
427 air quality missions will serve as a traveling standard for the inter-comparability of the different  
428 GEO instruments. Further efforts should focus on the development of an harmonized framework  
429 for the processing, validation, and publication of all data products from the constellation of GEO  
430 composition observations (CEOS 2019).

431 The availability of multiple measurements per day also provides opportunities for improved  
432 retrieval techniques. For example, the nearly simultaneous observation of contiguous scenes  
433 facilitates cloud slicing, where differences in column amounts above optically thick clouds are used  
434 to provide information on vertical distribution (Marais et al. 2021). Imagers and spectrometers on  
435 GEO platforms, combined with LEO missions, will deliver measurements of multiple chemical  
436 species over emission hotspots across a broad spectral range. This expanded coverage has the  
437 potential to enable the retrieval of new information and deepen our understanding of emission  
438 activities.

### 439 *b. Modeling*

440 GEO composition observations will be useful for the evaluation of high-resolution regional and  
441 local chemical transport models, and specifically to compare calculated diurnal variations with the  
442 hourly data provided by the retrievals. The measured variations in column concentrations may be  
443 very different from the time evolution of surface concentrations (e.g., Tang et al. 2021). A full  
444 understanding of the observed diurnal variation is not straightforward because, in addition to the  
445 time-evolving forcing from solar radiation, it is driven by other factors such as local emissions,  
446 boundary layer meteorology, etc. (Edwards et al. 2024). One challenge is to improve the represen-  
447 tation of small-scale dynamical features in the planetary boundary layer, including the formation of

the heat island in urban areas, the development of convective cells and local cloudiness, the impact of topography and buildings on the small-scale flow, and the influence of diurnal varying coastal circulation cells.

Regional chemical-meteorological models at a spatial resolution of typically 1 to 5 km are used to provide background information on the chemical composition; they are now often complemented by numerical simulations of large eddies in the boundary layer in order to resolve their impact on the reaction rates and on chemical segregation associated with emission heterogeneity in a complex urban canopy (Wang et al. 2022). Street network models such as the MUNICH model (Kim et al. 2018) provide the distribution of chemically reactive pollutants along street canyons. The success of such approaches depends on the availability of detailed high-resolution (better than 1 km) emission inventories, which are usually not yet available.

Recent efforts have led to the development of global multi-scale models with grid refinement capabilities over selected geographical regions. An irregular model grid with a grid refinement capability over the three regions covered by GEMS, TEMPO and Sentinel-4 has been developed as part of the next-generation community modeling infrastructure, MUSICA (the Multi-Scale Infrastructure for Chemistry and Aerosols; Pfister et al. 2020). Its purpose is to insert high-resolution regional information provided by the GEO satellites in a global modeling framework that accounts for large-scale transport and distant influences on chemical species (Pfister et al. 2020).

### *c. Data assimilation*

There are several challenges related to the assimilation of GEO observations. The efficient assimilation of such dense observations will require high-resolution forecast models and appropriate data assimilation techniques, in addition to a flexible system handling multiple satellite sensors from both GEO and LEO. As summarized below, further innovations are needed to take advantage of GEO satellite observations with data assimilation.

(1) Parameter estimation: In tropospheric chemistry, boundary conditions, reaction rates, and emissions often play an important role, whereas the role of initial conditions is limited due to rapid chemical reactions (Sandu and Chai 2011; Goris and Elbern 2013). Dense observations from GEO satellites may allow for detailed parameter estimation beyond a few key chemical species, improved

sectoral emissions estimates (Qu et al. 2022a; Gaubert et al. 2023), and speciation information for VOCs and aerosols. They can also be used to correct for meteorological parameters such as horizontal wind (Liu et al. 2021).

(2) Data assimilation methodology: With greater observational coverage and high measurement accuracy, local emission sources could be estimated using computationally efficient approaches such as the mass balance approach (e.g., Cooper et al. 2017; Qu et al. 2019), or by making use of trajectories to describe the non-local relation between emissions and concentrations (e.g., van der A et al. 2024). Nevertheless, flow-dependent background covariance, including covariance among chemical species, is essential to integrate multiple-species information and their spatial distributions. DA techniques also need to account for diurnal changes in chemistry, emissions, and measurement characteristics (e.g., Timmermans et al. 2019; Shu et al. 2023). Efficient non-Gaussian methods such as particle filters may also be needed for high-resolution DA (Valmassoi et al. 2023).

(3) Plume analysis and emission estimates: The latest GEO and LEO satellite composition observations are able to resolve plumes of urban emissions, major point sources and even individual ships. Computationally efficient techniques such as plume fitting (e.g., Fioletov et al. 2017), the flux-divergence technique (e.g., Beirle et al. 2023), or the integrated mass enhancement method (e.g., Varon et al. 2018; He et al. 2024a) have been successful in providing emission estimates for short-lived and long-lived tracers at the instrumental resolution. A major challenge for short-lived compounds like  $\text{NO}_2$  is to account for the non-linear chemistry in plumes, leading to a heterogeneous plume composition and lifetime (Krol et al. 2024), and to determine how these local effects impact global or regional data assimilation systems.

(4) Combination of multiple observing systems: LEO composition observations provide constraints on long-range transport (Miyazaki et al. 2022) and reduce model errors in regions constrained by GEO composition observations. Well-validated LEO data can be used to benchmark GEO composition observations, for example, as an anchor for DA bias correction. As the spatial resolution of both forecast models and satellites increases, assimilation of in situ and satellite observations will be another effective approach to improve analysis, especially near the surface. New technical challenges for simultaneous assimilation include appropriate background error co-



506 variance at multiple scales and error statistics including representative errors of each measurement  
507 (Wang and Wang 2023).

#### 508 *d. Machine learning*

509 For future applications of machine learning in air quality research, the differences between LEO  
510 and GEO viewing geometries need to be accounted for. Solar zenith angle and viewing zenith  
511 angle could have greater importance when constructing machine learning models for retrieving  
512 atmospheric composition from GEO satellites. Diurnal variations in related physical parameters  
513 should also be captured by input variables for machine learning models for GEO composition  
514 satellites.

515 Recent applications of machine learning for LEO atmospheric composition satellites have focused  
516 on concentration estimation and the development of surrogate models. More efforts are needed in  
517 applying machine learning to inverse modeling of emissions. Specifically, further development of  
518 explainable machine learning models is necessary to enhance the interpretability and robustness  
519 of emission estimates.

520 Despite the challenges, geostationary atmospheric composition satellites offer opportunities to  
521 further advance innovation in future machine learning applications. For example, machine learning  
522 is effective in anomaly detection and pattern recognition, both making it well-suited for monitoring  
523 extreme events (e.g., wildfires and volcano eruptions). Its scalability to the high temporal and  
524 spatial resolution of GEO composition measurements can be critical for real-time decision-making  
525 and mitigating the impacts of extreme events.

526 The generalizability of machine learning is another key strength that enhances data fusion.  
527 Recent studies indicate that integrating multi-source measurements using machine learning can  
528 help reduce discrepancies between different datasets (Balasus et al. 2023; Oak et al. 2024; Huang  
529 et al. 2024). Integrating LEO composition measurements can play a critical role in improving the  
530 consistency of composition measurements made by different GEO satellites.

#### 531 *e. Atmospheric composition monitoring for other regions of the world*

532 Space-borne instruments in LEO have been vital for addressing data sparsity in large parts of  
533 the world, in particular for the African and South American continents and parts of Asia. These

regions will continue to rely on LEO instruments, as the planned GEO satellite constellation mainly covers the Northern Hemisphere (Paton-Walsh et al. 2022). The validation of both LEO and GEO observations and the derived products is also rare across the tropics and Southern Hemisphere. Such validation requires routine surface observations and aircraft campaigns to profile the troposphere under a range of representative conditions (Tang et al. 2023).

The Sentinel-4 GEO composition instrument will observe a portion of North Africa, and the IRS on the same platform will provide observations of infrared-absorbing compounds like CO and NH<sub>3</sub>. CO observations over Africa will be vital for understanding inefficient combustion sources, including biomass burning for agricultural practices in Africa (Andreae 2019), burning of waste (Wiedinmyer et al. 2014), and from other inefficient combustion practices (Marais and Wiedinmyer 2016; Bockarie et al. 2020). High-frequency NH<sub>3</sub> observations are well timed to coincide with agricultural intensification that includes the use of synthetic nitrogen fertilizer and intensive livestock farming (Hickman et al. 2021). A demonstration of the utility of GEO observations of NH<sub>3</sub> and CO for informing diurnal changes in abundances, precursor emissions, and pollution transport patterns over Africa would aid in advocating for dedicated GEO instruments over Africa and South America. However, the long delay between mission concept and launch means missing out on advancing understanding in regions of the world during a period of unprecedented population growth and land use changes. An advisory committee comprising researchers, academics and satellite instrument developers has been formed to propose GEO missions over Africa and South America, but a greater representation of researchers from these regions is needed to inform the development of a fit-for-purpose mission (Marais and Chance 2015).

## 5. Conclusions and recommendations

The implementation of GEO satellites for atmospheric composition monitoring opens new perspectives for air quality research. The first two GEO composition satellites over Asia and North America have demonstrated the measurement of diurnal variation of chemical species, thereby providing unprecedented information on the diel evolution of emissions, photochemical processes and the effects of atmospheric dynamics over large regions. However, the development of retrievals and the validation of these GEO satellite composition data is still ongoing, as there is still room for improvement. Furthermore, the European component of the GEO constellation in Sentinel-4 is

563 expected to be launched in 2025. The exploitation of measurements conducted by GEO satellites  
564 presents new challenges and several priority tasks can therefore be highlighted for future research.

- 565 • Retrieval algorithms need to be carefully adapted to the GEO composition observations.  
566 Specifically, the diurnal variations of various parameters used in the retrieval, such as surface  
567 reflectivity and vertical mixing, need to be resolved. Additionally, the viewing geometry can  
568 present difficulties due to the large zenith angles of GEO instruments compared to nadir-  
569 viewing satellites, hence correcting for these effects at the edges of the field of regard is  
570 necessary.
- 571 • The hourly temporal resolution of GEO observations gives crucial information on diurnal  
572 profiles of emissions of atmospheric pollutants. In order to leverage this aspect in emission  
573 inversion studies and reduce the delay in the delivery of emission inventories, temporal profiles  
574 for different sectors in emission inventories need to be provided.
- 575 • Global and regional models should be adapted to be more compatible with the GEO at-  
576 mospheric composition satellites. Continuous model development, especially regarding the  
577 fine-scale chemical processes, is essential for retrievals, air quality forecasting, and data  
578 assimilation in the era of GEO satellites for atmospheric composition monitoring.
- 579 • Data assimilation methods need to be adapted to the geostationary case. Specifically, more  
580 computationally efficient methods should be explored in order to optimally process the high  
581 data volume. The co-existence of LEO and GEO measurements in the same area opens  
582 possibilities to assimilate both datasets simultaneously, along with ground-based and aircraft  
583 data. Deriving emissions from point sources from plume estimation methods also provides a  
584 promising avenue, considering the higher temporal resolution of observations.
- 585 • The computational efficiency and generalizability of machine learning make it a valuable  
586 area for further exploration. In addition to recent applications of machine learning in retrieval  
587 algorithm development and surface concentration estimation, greater efforts should be directed  
588 toward inverse modeling of emissions and the development of explainable models.

589 Finally, it is crucial to keep improving the accessibility of satellite measurements to agencies  
590 in charge of air quality management, especially for regions lacking the capability to establish

591 observation networks. Future GEO satellites should provide data over Africa, South America,  
592 Southern Asia, Australia, New Zealand, and other regions not covered by the current observing  
593 capabilities.

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The GEMS NO<sub>2</sub> tropospheric column density data are publicly available on request from the National Institute of Environmental Research (NIER) Environmental Satellite Center (ESC) ([https://nesc.nier.go.kr/en/html/datasvc/data.do?pageIndex=1&outputInnb=64&atrb=NO2\\_Trop](https://nesc.nier.go.kr/en/html/datasvc/data.do?pageIndex=1&outputInnb=64&atrb=NO2_Trop), last access: 3 August 2024). The TEMPO NO<sub>2</sub> tropospheric columns are openly available from the NASA Earthdata Atmospheric Science Data Center ([https://asdc.larc.nasa.gov/project/TEMPO/TEMPO\\_NO2\\_L2\\_V01](https://asdc.larc.nasa.gov/project/TEMPO/TEMPO_NO2_L2_V01) with DOI:10.5067/IS-40e/TEMPO/NO2\_L2.001, last access: 3 August 2024). The TROPOMI monthly mean NO<sub>2</sub> tropospheric columns are available from the KNMI Tropospheric Emission Monitoring Internet Service ([https://www.temis.nl/airpollution/no2col/no2month\\_tropomi.php](https://www.temis.nl/airpollution/no2col/no2month_tropomi.php), last access: 3 August 2024).

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