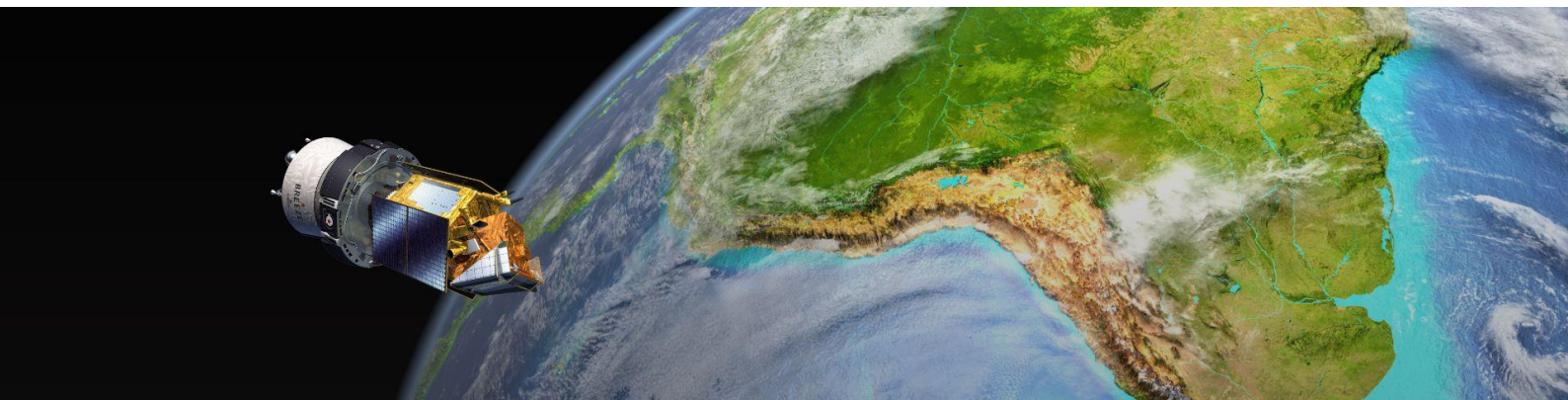


Satellite-based Air Pollution and Greenhouse Gas Monitoring in Uruguay



TNO 2024 R10400 – 2 April 2024

Satellite-based Air Pollution and Greenhouse Gas Monitoring in Uruguay

Author(s)	Jerry Ge, Ioanna Skoulidou
Classification report	TNO Public
Title	TNO Public
Report text	TNO Public
Appendices	TNO Public
Number of pages	26 (excl. front and back cover)
Number of appendices	3
Project name	Uruguay - Trompomi Phase 1 Feasibility
Project number	060.54613

All rights reserved

No part of this publication may be reproduced and/or published by print, photoprint, microfilm or any other means without the previous written consent of TNO.

© 2024 TNO

Summary

To strengthen the capacity to monitor air quality at the national level using satellite data and emission inventory, the Environmental Information Division of the Ministry of the Environment of Uruguay asked TNO to provide an initial assessment of the availability, quality, and feasibility of using satellite observations and chemistry transport models (CTMs) for air pollution and greenhouse gas monitoring in Uruguay.

In this assessment, TNO has used a combination of satellite information (e.g. Sentinel-5P) and its LOTOS-EUROS model to assess air pollution and greenhouse gas levels in Uruguay and identify their contributing sources. The conclusion shows that satellite data and chemistry transport models can help to address the following air quality challenges:

1. Forest fire emissions are underestimated in inventories that are normally used for air quality prediction.
2. The emission inventory of Uruguay is not always complete in terms of emission sources.
3. The contribution of air pollutants from outside the country is unclear, e.g. from big cities like Buenos Aires and sudden sources like volcanoes.
4. There is a lack of ground station coverage in some parts of the country.

The assessment shows that satellite-based air pollution and greenhouse gas monitoring can contribute to several benefits:

1. Improve early warning alerts e.g. smog for people with chronic obstructive pulmonary disease.
2. Better understand the contribution of local pollution sources to air pollution in Uruguay and where mitigation actions in Uruguay are justifiable.
3. Better understand the contribution of transboundary pollution sources, when and how strongly they affect air pollution in Uruguay, allowing for improved accuracy of predictions.
4. Get air quality readings in areas where ground infrastructure is lacking while saving money on ground infrastructure expansion, maintenance, and operations.

A key example of the added value of satellite-based monitoring of air pollutant levels is illustrated in figure 1.1.

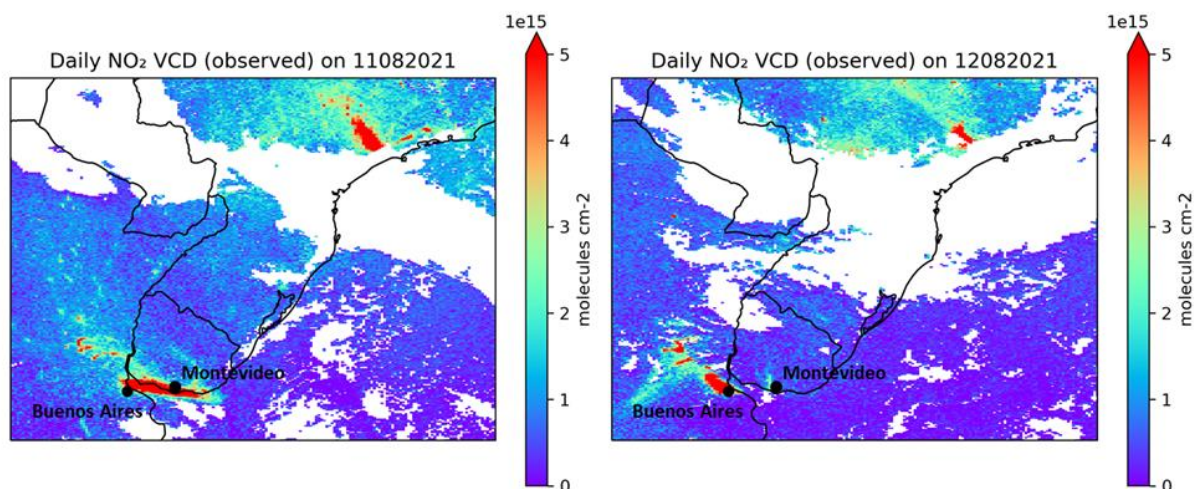


Figure 1.1: Daily average of NO₂ vertical column density observed over Uruguay on 11/08/2021 (left) and 12/08/2021 (right). Each image is composed of two satellite passes.

This figure 1.1 shows the daily average of NO₂ vertical column density observed over Uruguay on 11/08/2021 and 12/08/2021 from the Sentinel-5P satellite. Each image is composed of two satellite passes. One can see that on 11/08/2021, the NO₂ plume from Buenos Aires reached all the way to Montevideo, having a negative impact on the air quality over the most populated area in Uruguay. However, due to different wind directions on the next day, the plume changed directions and Uruguay is free from the air pollutant from outside the country. This example emphasizes the importance of developing a real-time air pollution system that can incorporate satellite data, a chemistry transport model, existing emission inventories, and in-situ ground monitoring infrastructure in Uruguay.

Contents

Summary	3
Contents	5
1 Introduction	6
2 Methodology and data	7
2.1 Methodology	7
2.2 LOTOS-EUROS coupled with CSO	8
2.3 The CAMS Global Fire Assimilation System (GFAS) emissions	8
2.4 Emissions Database for Global Atmospheric Research (EDGAR)	9
2.5 Sentinel-5P / TROPOMI	9
3 Results	10
3.1 NO ₂ vertical column density	10
3.1.1 Annual averaged NO ₂ total columns	10
3.1.2 Monthly averaged NO ₂ total columns during fire season in August	12
3.1.3 Unique events	13
3.2 SO ₂ vertical column density	15
3.3 CH ₄ total column-average dry-air mixing ratio	16
4 Conclusions	18
5 Recommendation	19
6 References	21
Signature	22
Appendices	
Appendix A: Background: Emission of Air Pollution and Methane	23
Appendix B: The CAMS Satellite Operator	24
Appendix C: Filtering criteria of NO ₂ , SO ₂ and CH ₄ from Sentinel-5P observations	26

1 Introduction

The overall goal of this study is to provide an assessment of the availability, quality, and feasibility of using satellite data and chemistry transport models to improve air pollution and greenhouse gas monitoring in Uruguay, specifically emission identification linked to waste management at final disposal sites and forest fires¹. This will be done by focusing on the following:

- › Observations from the Sentinel-5P satellite of the European Space Agency (ESA) for the pollutants NO₂, SO₂, and CH₄
- › Use of the open-source chemistry transport model LOTOS-EUROS of TNO to predict the dispersion of pollutants at the local, national, and regional level
- › Copernicus GFAS product (fire emission) over Uruguay, which is derived using satellite imagery.

This study is undertaken in the context of establishing cooperation between the Ministry of the Environment and TNO to strengthen the capacity of the Ministry to monitor air quality. TNO is an independent research organization from the Netherlands, which builds satellite instruments for air pollution monitoring e.g. for ESA and NASA, and whose LOTOS-EUROS model is used in the Copernicus Atmosphere Monitoring Service (CAMS) for European air quality prediction on a daily basis. The study for the Ministry will help address how best practices from CAMS and Europe can be applied in Uruguay. It anticipates the possibility of starting a process of developing and implementing a (real-time as well as forecasting) system for air quality management, using satellite data and simulation models. In addition, TNO has also provided the LOTOS-EUROS model and training in its use to employees of the Ministry.

¹ A short description on the background of air pollution and greenhouse gas emissions can be found in Appendix A

2 Methodology and data

2.1 Methodology

Fire emissions from the GFAS (the CAMS Global Fire Assimilation System, see Section 2.3) inventory and anthropogenic emissions from EDGAR (Emissions Database for Global Atmospheric Research, see Section 0) were used in the chemistry transport model LOTOS-EUROS to derive vertical column densities (VCDs) of air pollutants. Coupled with vertical column density measurements from satellite Sentinel-5P, we were able to investigate the emission inventories and the satellite's capabilities to detect air pollutant concentrations caused by fires and landfills.

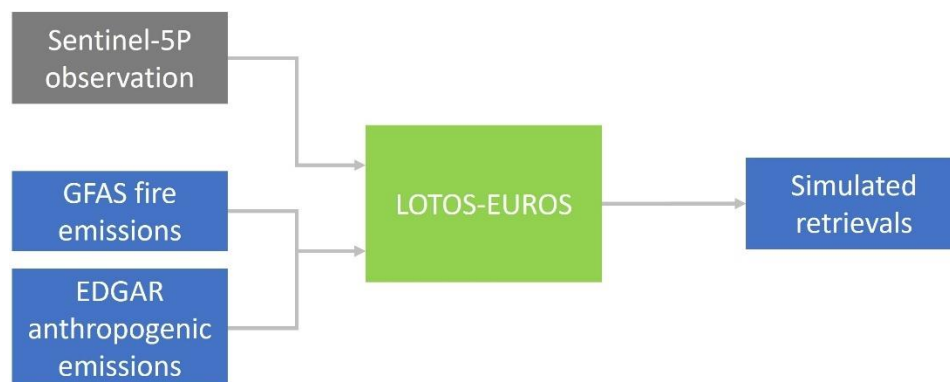


Figure 2.1: A simplified overview of using GFAS emission data to simulate total columns of NO₂, SO₂ from forest fires, and CH₄ from landfills.

Figure 2.1 illustrates the simplified overview of how to use GFAS emission data and Sentinel-5P observations to monitor air pollutants from forest fires and landfill sites, which was conducted in the following steps:

1. Find seasons and events that are representative of forest fire and landfill emissions through reports, news, and registries.
2. Download, convert, and list Sentinel-5P observations using CAMS Satellite Operator (CSO) after defining the spatial and temporal domain, as well as the filtering criteria.
3. Run LOTOS-EUROS for the given spatial and temporal domains, coupled with CSO format Sentinel-5P observations to derive simulated retrievals using model variables.
4. Compare simulated total columns with simulated retrievals and determine whether the fire emission inventory and Sentinel-5P observations can identify fire events and landfill sites.

2.2 LOTOS-EUROS coupled with CSO

The LOTOS-EUROS model is an Eulerian chemistry transport model that simulates air pollution in the lower troposphere. In this project, the spatial resolution of LOTOS-EUROS was set to 0.125° in longitude and 0.0625° in latitude. The model's physical processes include advection, diffusion, dry and wet deposition, chemistry reaction, and sedimentation. LOTOS-EUROS uses a set of temporal factors (monthly, daily, and hourly) to break down annual total emissions into hourly emissions. LOTOS-EUROS has been used for a wide range of applications supporting scientific research. It is used for daily operational air quality forecasts over Europe and the Netherlands, as well as for daily forecasts of dust concentrations over North Africa, and the forecast of dust storms in China.

The observation operator from CAMS Satellite Operator (details in appendix b) has been incorporated into the LOTOS-EUROS output modules. Within this project, LE version v2.2.003 was run at a resolution of 0.125 degrees x 0.0625 degrees, with decomposition into horizontal subdomains when running in parallel. The horizontal mapping tool from CSO was used to average simulated output over the footprint area. In the vertical, 12 layers were used, which are a coarsening of the ECMWF meteorological layers (L137), with a top of around 300 hPa or 10 km. To simulate satellite observations, a user-defined number of layers could be added on top of the model to fill the entire atmosphere; their concentrations are taken from global boundary conditions (usually CAMS/IFS simulations). After averaging over the footprint, the pressure profile of the model is scaled such that it has a surface pressure equal to that defined in the retrieval product; this could be used to ensure that the total tracer mass in a column remains the same after mapping to the retrieval layers.

2.3 The CAMS Global Fire Assimilation System (GFAS) emissions

We used the CAMS Global Fire Assimilation System (GFAS) emission inventory, which assimilates fire radiative power (FRP) observations from satellite-based sensors to produce daily estimates of wildfire and biomass burning emissions (Kaiser et al. 2012). The GFAS data output includes spatially gridded Fire Radiative Power (FRP), dry matter burnt, and biomass burning emissions for a large set of chemicals, greenhouse gases, and aerosol species. The FRP and biome-specific conversion factor are multiplied to estimate the burned biomass and derive fire emissions. FRP observations currently assimilated in CAMS GFAS are the NASA Terra MODIS and Aqua MODIS active fire products (<http://modis-fire.umd.edu/>). Data are available globally on a regular latitude-longitude grid with a horizontal resolution of 0.1 degrees from 2003 to the present.

2.4 Emissions Database for Global Atmospheric Research (EDGAR)

The Emissions Database for Global Atmospheric Research (EDGAR) provides global gridded anthropogenic emissions of greenhouse gases and air pollutants, using spatial proxy datasets with the location of energy and manufacturing facilities, road networks, shipping routes, human and animal population density, and agricultural land use (Crippa et al. 2018). Input datasets (point, line, and area grids at various resolutions) to EDGAR are annual statistics, which are resampled and aggregated onto a 0.1°x0.1° grid. National sector totals are distributed using the spatial proxies over the country's area and sector- and region-specific monthly profiles are applied to generate global monthly emission grid maps.

2.5 Sentinel-5P / TROPOMI

Launched in 2017, Sentinel-5P is a part of the European Union's Copernicus Program, which aims at delivering timely and quality data about our environment. Its onboard primary instrument, TROPOMI (Tropo-spheric Monitoring Instrument), is a spectrometer that detects the sunlight reflected off Earth's surface and offers detailed observations of the concentrations of various atmospheric components, including NO₂, SO₂, and CH₄.

Using TROPOMI observations has the following advantages. Firstly, TROPOMI's high resolution (5.5km x 3.5km at nadir for NO₂ and SO₂, 5.5km x 7km at nadir for CH₄) enables the identification of local emission hotspots, a key advantage in pinpointing specific sources of pollution in Uruguay. Secondly, Sentinel-5P provides daily global coverage, allowing for real-time tracking of emission sources. This can be crucial for early intervention during forest fires and to ensure that landfill emissions are within acceptable limits. Lastly, the data is freely accessible, promoting transparency and facilitating scientific research.

There are also difficulties. Besides clouds' negative impact on measuring air pollutant levels, it is also a challenge to relate satellite observations to surface-level concentrations. Several methods can convert satellite-based VCDs to surface concentrations, such as using chemistry transport model simulations. However, the method relies on a surface-to-column ratio that converts satellite-observed vertical columns into surface concentrations. However, the vertical profiles and surface-to-column ratios need to be further studied for Uruguay.

We used the CAMS Satellite Operator (CSO) to download and process the TROPOMI data (details in appendix b). It has to be pointed out that data filtering criteria were applied to TROPOMI measurements of NO₂, SO₂, and CH₄ to ensure the quality of the data used. The filtering criteria are presented in appendix c.

3 Results

3.1 NO₂ vertical column density

In this section, we delve into the methodology of using Sentinel-5P to monitor NO₂ emissions from forest fires. Vertical column density indicates an integrated concentration metric over the entire atmospheric column. Simulated and retrieved VCDs were provided through LOTOS-EUROS using the emission inputs and the Sentinel-5P Level 2 products. By analyzing the spatial distribution of NO₂ VCD, areas with elevated concentrations can be identified. This is useful for pinpointing major emission sources or pollution events such as active fires.

Three temporal resolutions (and ranges) are chosen to test the emission inputs' and Sentinel-5P's capabilities to simulate NO₂ levels and identify fire events:

1. Annual averaged NO₂ total columns give a general perspective of the NO₂ level in the region and show how much fire emissions contribute to the annual average.
2. Monthly averaged NO₂ total columns during the fire season (August) illustrate how many fires the GFAS database can indicate.
3. Daily NO₂ total columns during unique events.

3.1.1 Annual averaged NO₂ total columns

The annual averaged NO₂ VCD from simulations and observations in 2021 are presented in figure 3.1. One can see that the simulated NO₂ levels match the observed ones well, with hotspots in large urban areas, such as Buenos Aires and Rosario in Argentina, and Sao Paulo and Rio de Janeiro in Brazil. However, some hotspots with relatively lower levels of NO₂ than urban areas in central Paraguay were missed. In addition, relatively higher levels of NO₂ appear along the Paraná River in Argentina in the observations (likely caused by ships), but they are not present in the simulation. Uruguay, compared to the surrounding countries, is much cleaner, with a much lower NO₂ VCD level and only relatively higher NO₂ VCD in the small region of the capital Montevideo. Besides, it is also clear that the NO₂ coming from Buenos Aires can have an impact on the NO₂ level in Uruguay since the city of Buenos Aires is a large source of NO_x and is located very close to the border.

Figure 3.2 shows the time series of observed and simulated NO₂ VCD in Buenos Aires and Montevideo. It is shown that the timings of the peaks are simulated quite well but the magnitudes of the peaks sometimes are off. The mismatch in magnitude is especially evident in January, April, and August. Commonly, there are more fires in January and August because of the hot summer and dry winter. Besides, Decree N° 436 of Uruguay regulates that during the period between 1st December to the second week of April, it is forbidden to conduct agricultural burnings. It is possible that right after the forbidden period, agricultural burnings were conducted. This means that the fire emissions from GFAS have larger uncertainties during fire seasons. It highlights the necessity for updated and more accurate real-time emissions and also a case of satellite monitoring during the fire seasons.

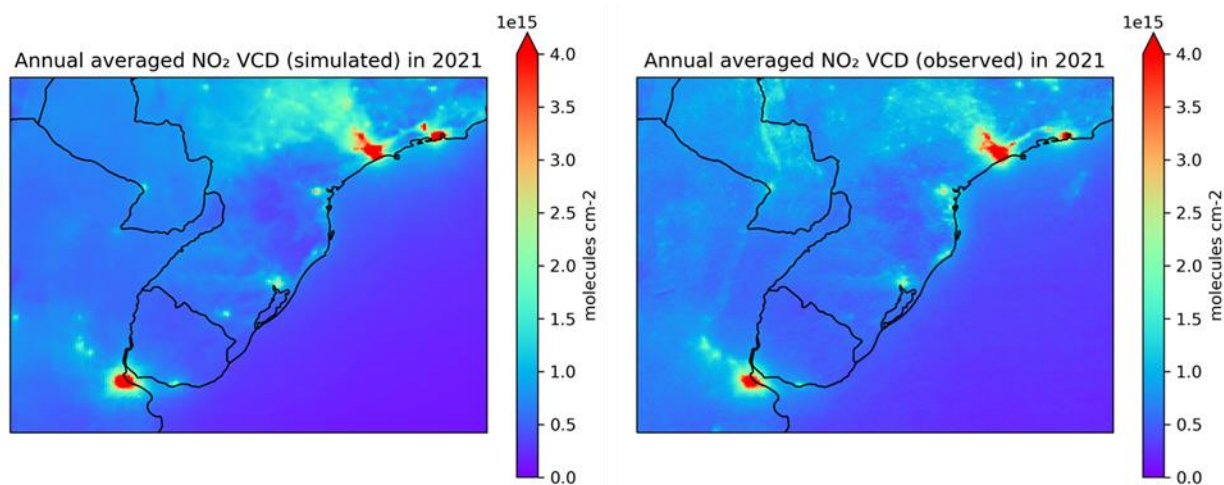


Figure 3.1: Simulated (left) and observed (right) annual averaged NO₂ vertical column density in 2021.

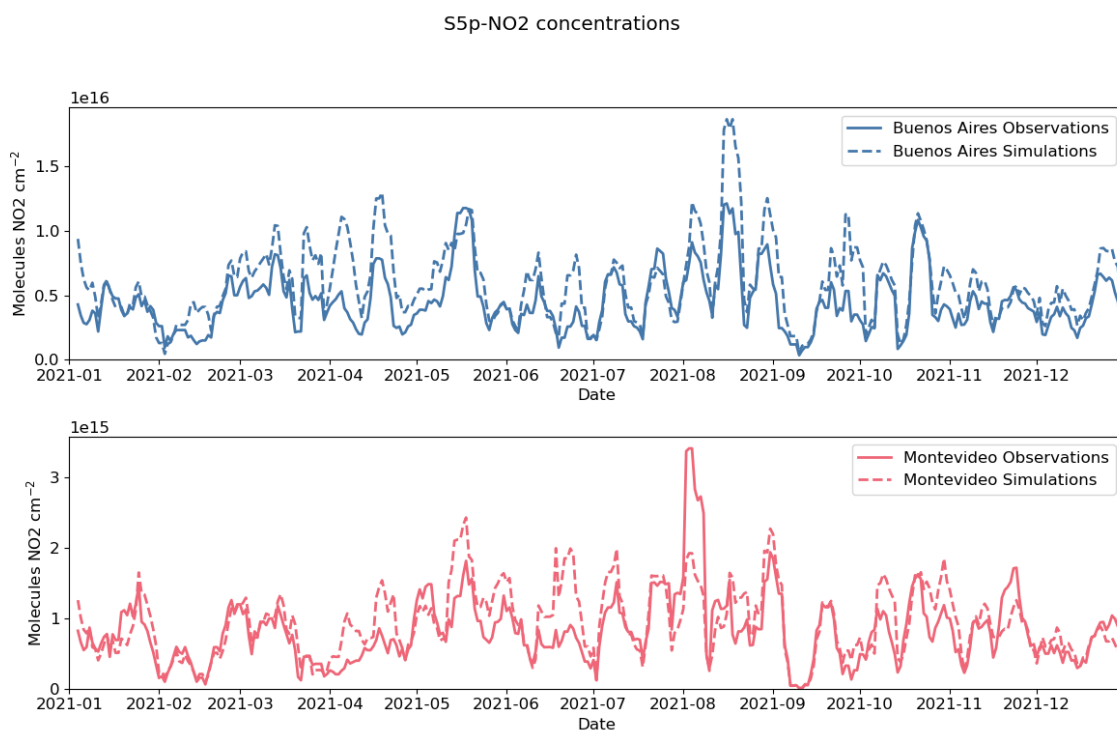


Figure 3.2: Time series of simulated and observed NO₂ vertical column density in Buenos Aires and Montevideo in 2021.

3.1.2 Monthly averaged NO_2 total columns during fire season in August

As is shown in figure 3.2, the difference between the simulations and observations is the highest in August, which is among the typical fire seasons in the region. The comparison of monthly averaged simulated total columns and retrievals in August is shown in figure 3.3. The NO_2 level in Uruguay is again very low in both simulations and observations. It is apparent that even though the model still simulated the NO_2 VCD levels in urban areas pretty well, it missed large hotspots in Paraguay and Argentina, which were caused by emissions taking place between 16 – 23 August 2021 (one example of 18 August shown in figure 3.4). The observed NO_2 VCD hotspots on 18 August in Paraguay correspond with the fire events derived from NASA Fire Information for Resource Management System (FIRMS) in figure: 3.5. The GFAS emission input should be investigated, which is presented in Section 3.1.3.

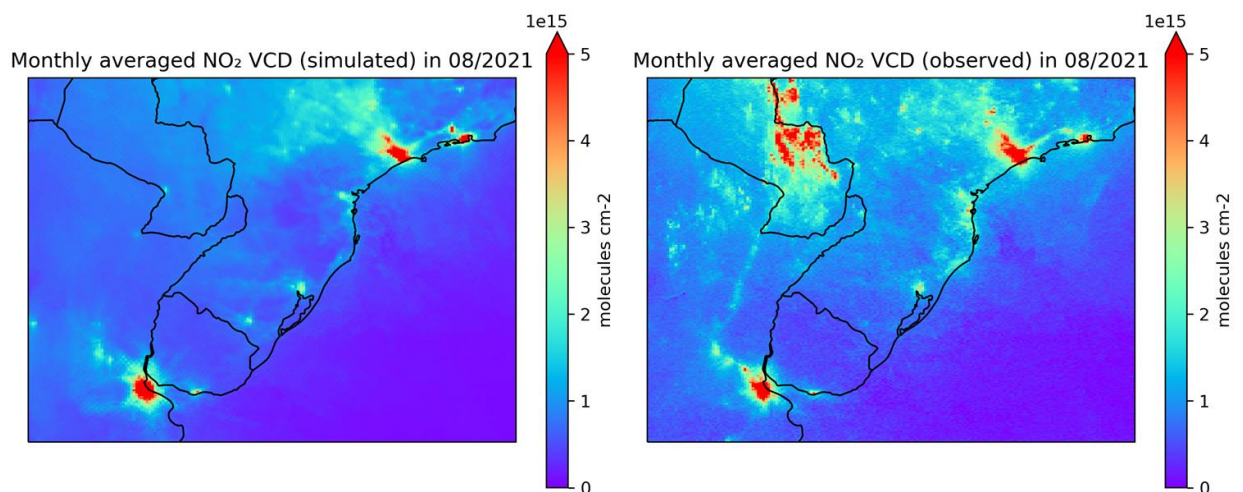


Figure 3.3: Simulated (left) and observed (right) monthly averaged NO_2 vertical column density in August 2021.

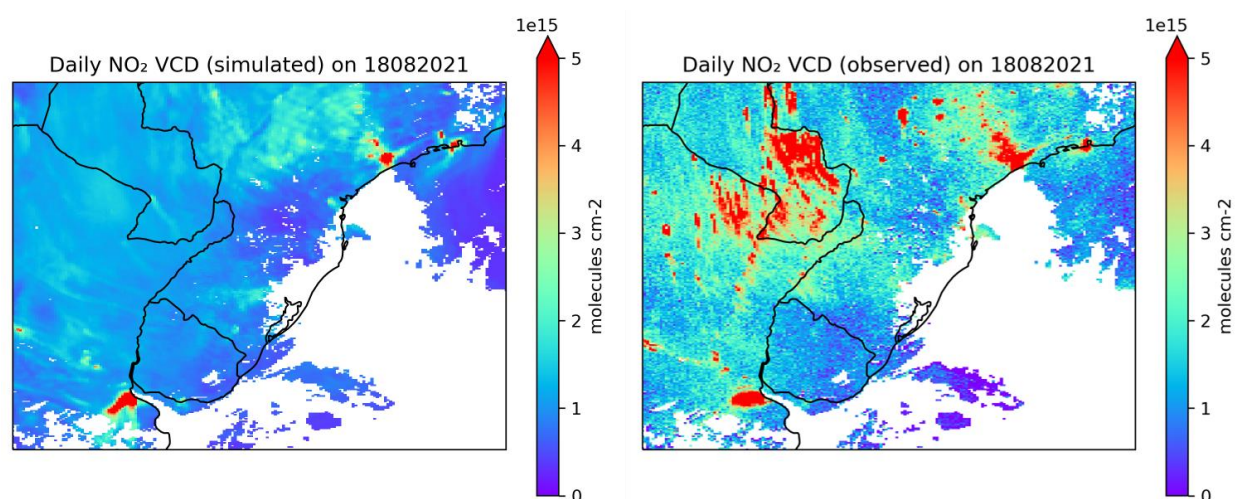


Figure 3.4: Simulated (left) and observed (right) NO_2 vertical column density on 18 August 2021.

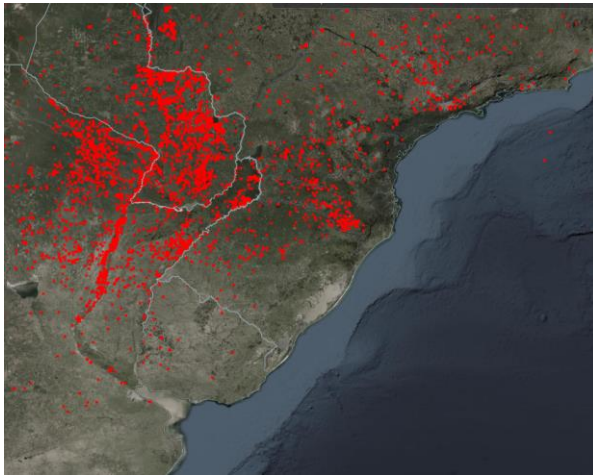


Figure: 3.5 Fire locations on 18 August 2021 from NASA Fire Information for Resource Management System (FIRMS).

3.1.3 Unique events

According to press reports, on Wednesday, December 29, 2021, a fire started in the department of Río Negro when a truck caught fire. The fire spread through the surrounding grasslands and mountains, arriving at the town of Algorta. In the following days, the fires continued to advance through the area, affecting the towns of Algorta, Piedras Coloradas, Orgoroso, Pandule, and Menaфра. The light blue area in figure 3.6. A forest fire was observed in the southwest of the department of Río Negro in the vicinity of Esteros de Farrapos, affecting the Municipality of San Javier, which is marked in the yellow zone in figure 3.6. It is said to be the largest fire in recent years in Uruguay. It is a suitable test case for fire monitoring.

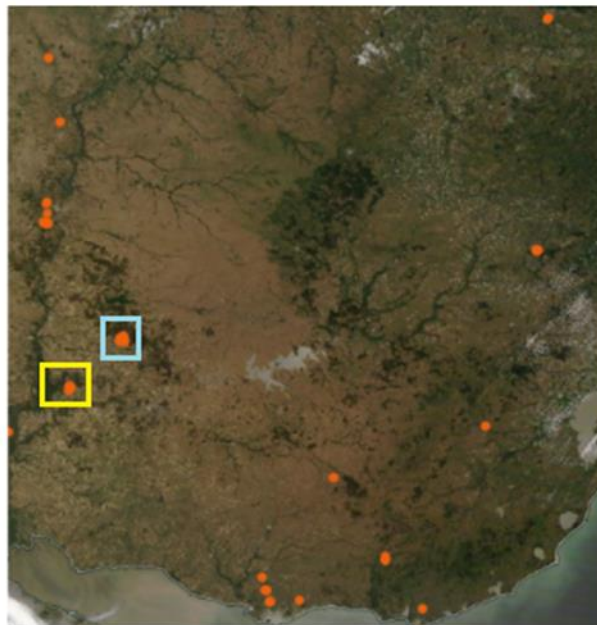


Figure 3.6: Fire detection according to MODIS satellite platforms on December 30, 2021.

As a result, the NO₂ VCD maps on 31 December 2021 from simulations and observations are shown in figure 3.7. In the region where the fire broke out, Rio Negro – Paysandu (marked as light blue and yellow zones in figure 3.6), NO₂ VCD hotspots can be seen in the observations. However, they are not visible in the modeled results.

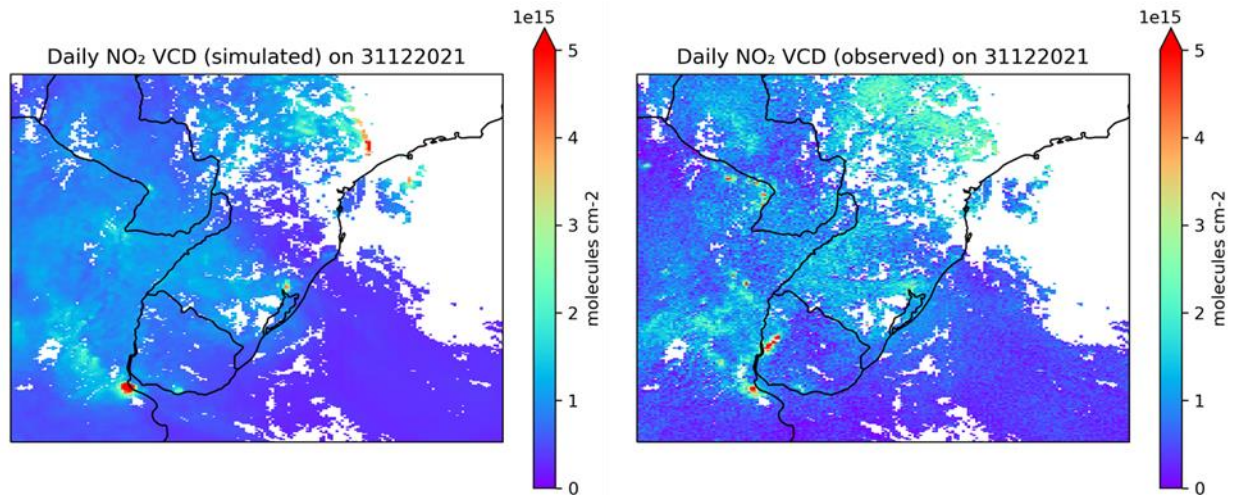


Figure 3.7: The comparison of simulated retrievals and simulated total columns during the Rio Negro - Paysandu fire event.

Subsequently, the GFAS emission input was investigated for 31/12/2021 (Rio Negro – Paysandu) and 18/08/2021 (in figure 3.4). The NO₂ fire emission maps on these two days are demonstrated in figure 3.8. One can see that the GFAS managed to estimate the location of the fire, with the hotspot corresponding to VCD hotspots from Sentinel-5P observations. However, these emission hotspots are not visible in the model VCD output. Just as Xue et al. (2024) pointed out, GFAS have uncertainties in estimating fire-burned areas and emissions and may underestimate emissions of wildfires, leading to the model's inability to reproduce the hotspots and plumes shown in the satellite measurements over Uruguay, especially during the fire sea-sons or unique events.

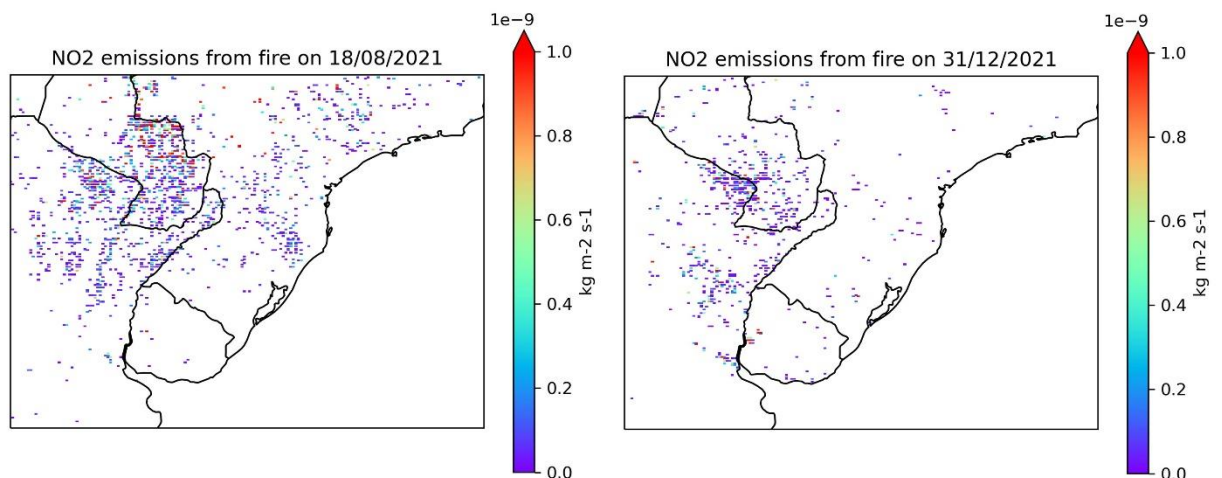


Figure 3.8: NO₂ fire emission from GFAS in Uruguay on 31/12/2021 (left) and surrounding Uruguay on 18/08/2021 (right).

There are alternative fire emission databases that could provide better fire emission estimates for South America. For example, the Fire Inventory from the National Center for Atmospheric Research (NCAR) version 2.5 (FINNV2.5) includes numerous updates such as better representing burned areas, vegetation burned, and chemicals emitted, allowing smaller fires to be included in the emissions processing (Wiedinmyer et al. 2023). However, it is shown that uncertainties in the emissions estimates remain, particularly in South America during August–October after investigating the performance of FINNV2.5 emissions as inputs to a CTM and assessing with satellite observations.

To have a better estimate of fire emissions and detect emission sources, we can use assimilation techniques with satellite data. Assimilation techniques offer significant prospects for enhancing the accuracy of emissions mapping both temporally and spatially. By integrating satellite data with appropriate inverse models, we can estimate emission fluxes, pinpoint regions of high emissions on a global level, and impose top-down limitations on emission estimates.

3.2 SO₂ vertical column density

SO₂ retrievals have a rather low signal-to-noise ratio, making the validation of SO₂ emission and VCD through satellite observations challenging. To better demonstrate and compare SO₂ VCDs, different colormaps are used in figure 3.9 to ‘remove’ the background SO₂ noise in the observations for visualization. The presence of noise is common in the current TROPOMI operational DOAS SO₂ retrievals. In general, Uruguay has a rather low background of SO₂, with higher values at a few locations only. The observations are much noisier than the modeled VCDs. Higher levels of SO₂ are observed in Uruguay over Montevideo and on the borders with Argentina and Brazil. The modeled results significantly underestimated SO₂ VCDs, which is caused by too low anthropogenic emission input from the EDGAR inventory, and/or too low SO₂ fire emissions from GFAS.

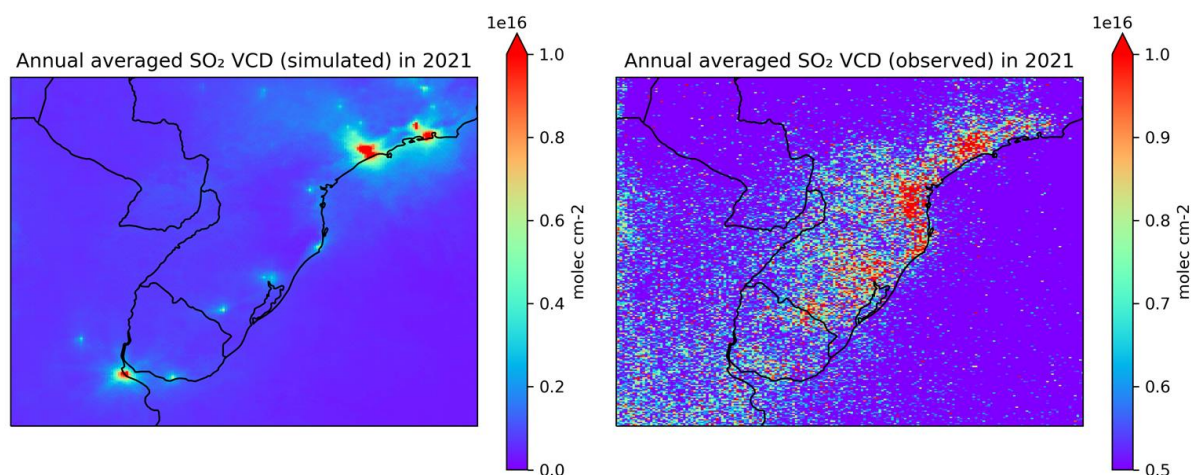


Figure 3.9: Simulated (left) and observed (right) annual averaged SO₂ vertical column density in 2021.

3.3 CH₄ total column-average dry-air mixing ratio

The potential emission sources of Methane (CH₄) include landfills, oil and natural gas systems, agricultural activities, coal mining, stationary and mobile combustion, wastewater treatment, and certain industrial processes. When the emission plume is strong enough, it might be visible in satellite data. However, the high background of concentrations hampers the isolation of emission plumes. The annual averaged CH₄ total column mixing ratio from simulations and observations is calculated and presented in figure 3.10. There are differences in the spatial patterns of CH₄ total column distributions. One can see that the simulated mixing ratios are generally slightly lower than the observed ones. This indicates that the background level of CH₄ that is obtained from global simulations is underestimated in the model. In addition, the simulation illustrates a gradient from south to north, while the observation shows a large hotspot in Buenos Aires (marked as 1) and more distinct column levels in Brazil (with gradients along the coastlines). The large hotspot in Buenos Aires was found to be caused by landfills (Maasackers et al. 2024). The more distinct CH₄ levels in Brazil are harder to link to an individual source. While the Rio Grande de Sul is known for cattle agriculture, the area in question is mostly wetlands and lakes, which can strongly affect the quality of the satellite retrieved concentrations. Regarding Uruguay, the current operational landfill sites are circled in figure 3.10. Both the simulations and observations show elevated CH₄ columns near some landfill sites in the south along the coast, as well as near the sites around Lago De Rincon Del Bonete (marked as 2) in the center of Uruguay. The sites around Lago De Rincon Del Bonete correspond to the national registry of landfills, which demonstrates the model's and observations' ability to detect emission sources. However, there are also a few hotspots next to Lago Andresito (marked as 3) and De Rincon Del Bonete, which are distant from registered landfill locations. There are two possible explanations. Firstly, this could be the result of emissions from other sources than landfills, for example, wetlands or fires. Secondly, similar to Rio Grande de Sul of Brazil, the water surfaces of lakes and wetlands hampers the quality of satellite retrievals. Here it should be kept in mind that due to the Sentinel-5P data selection criteria, the observations above the water of the Rio Negro have been filtered out. The quality and limitations of the data should also be acknowledged. Filtering on qa_value > 0.5 does not remove all pixels considered bad. Some pixels with too low methane concentrations are still present.

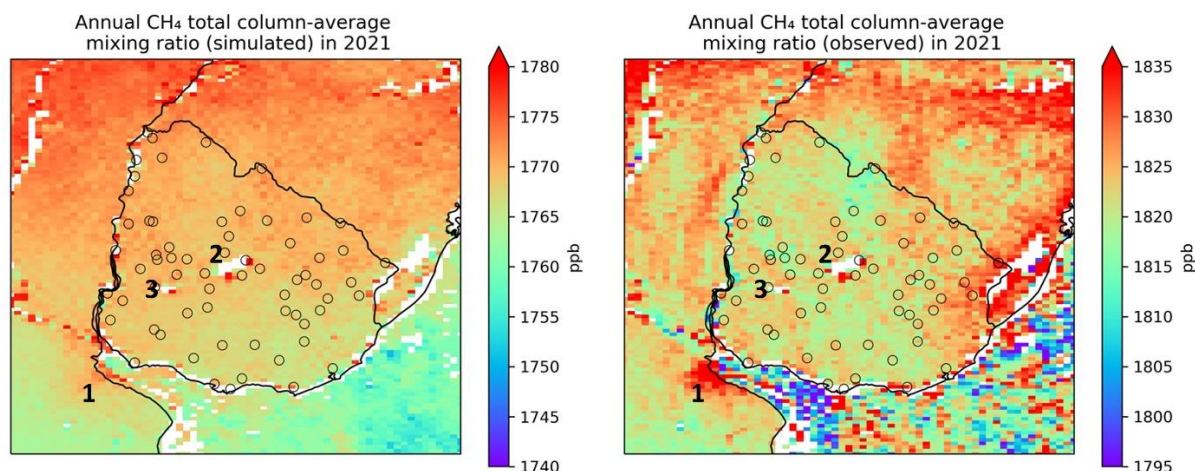


Figure 3.10: The comparison of annual-averaged simulated (left) and observed (right) CH₄ total column-average mixing ratios in 2021. Note that the color scales are different to correct for the too-low background values in the simulation. Buenos Aires is marked as 1, Lago De Rincon Del Bonete is marked as 2, and Lago Andresito is marked as 3.

To more accurately derive CH₄ emissions and quantify methane point source plumes, new techniques have been developed using multispectral 2 data from GHGSat, PRISMA, and Sentinel-2 (Schuit et al. 2023). These instruments have a spatial resolution of approximately 20-30 m. The SWIR bands measure the top-of-atmosphere radiance and are sensitive to methane absorption. They are useful for global monitoring emissions of large point sources and were applied in areas of known oil and gas activity (Gorroño et al. 2023). There have been studies using these observations to identify CH₄ emissions from landfills (Maasakkers et al. 2024).

4 Conclusions

The results obtained from this report show that:

- › Uruguay has generally low air pollution levels compared to the surrounding areas which have much larger sources such as urban areas and more forest fires.
- › Chemistry transport models such as LOTOS-EUROS and Sentinel-5P observations provide an approach to air quality forecasting and monitoring, but both have their advantages and limitations.
- › **Sentinel-5P is very useful in tracking emissions from sources like forest fires and landfill sites**, due to its high revisit time and spatial resolution. Its capabilities not only aid in understanding the immediate impact of such events on atmospheric composition, but also provide valuable insights into air pollutant distributions and trends through careful data selection, analysis, and validation.
- › **Modeling offers information on air quality with even higher spatial and temporal resolutions**. However, modeling relies on the quality of the emission inputs. GFAS can largely underestimate emissions from fire, resulting in missing air pollutant hotspots that are seen in observations. We also see that the emission inventory managed to pinpoint CH₄ sources from landfills very close to observations.

The current assessment represents the proof of concept of combining emission data, a regional-scale air quality model, and satellite information to assess and interpret air pollution levels in Uruguay and their contributors. These results show that the use of satellite data and chemistry transport models can be put to effective use in Uruguay. In the next section, we will provide recommendations on how their benefits could be realized.

5 Recommendation

Throughout the execution of this assessment, TNO found several air pollution monitoring challenges in Uruguay that can be addressed through satellite data and advanced simulation models. As a practical next step, TNO recommends developing a prototype of a real-time monitoring system that can demonstrate the added value for a selected number of air pollution challenges in close consultation with the end-user's needs within the Ministry. Such a prototype system will make available state-of-art solutions and best practices available in Uruguay like they are currently being developed and deployed in the Copernicus Atmosphere Monitoring Service (CAMS).

1. Forest fire emissions are underestimated in inventories that are normally used for air quality prediction.
Assimilation techniques offer significant prospects for enhancing the accuracy of emissions mapping both temporally and spatially. By integrating satellite data with appropriate inverse models, we can estimate emission fluxes, pinpoint regions of high emissions on a global level, and impose top-down limitations on emission estimates. Once the near-real-time fire emission estimates are improved, it is possible to provide early warning alerts e.g. smog for people with chronic obstructive pulmonary disease, etc.
2. Emission inventories in the region are not always complete in terms of emission sources. When anthropogenic emission inventories fail to take into account some emission sources, they usually result in emission products that overlook what is observed. The lack of information on emission sources not only causes estimate uncertainties in space and time but also hinders the understanding of the observations and physical and chemical processes. Anthropogenic emission inventories can be improved with detailed local input data such as land use. If so, the contribution of local pollution sources will be clearer and it will be much easier to determine where mitigation actions in Uruguay are justifiable.
3. The contribution of air pollutants from outside the country remains unclear, e.g. from big cities like Buenos Aires and sudden sources like volcanoes.
A better understanding of the origin of transboundary pollution can be created if known emission sources are labeled and tracked throughout LOTOS-EUROS to quantify transboundary pollution. Through this functionality, it is possible to determine how much percent of air pollutant concentrations come from different sectors and countries. However, this was not performed due to the scope constraints. In the meantime, better emission estimates using assimilation techniques can also help identify emissions from other countries including forest fires and large industrial areas.
4. There is a lack of ground station coverage in some parts of the country.
Although ground-based measurements usually have high temporal resolution, it is challenging to obtain continuous spatial coverage due to the discrete distribution of sites. The Sentinel-5P NO₂ total column product and auxiliary can be assimilated with meteorology data together to estimate surface NO₂ concentrations with wide spatial and temporal coverage. In this way, it is possible to get air quality readings in areas where ground infrastructure is lacking while saving money on ground-based infrastructure expansion, maintenance, and operations.

5. Using imagers with high spatial footprints to detect CH₄ sources and estimate emissions
For CH₄, new techniques have been developed to quantify methane point source plumes using imagers with high spatial footprints of approximately 20 m spatial resolution or better (e.g. Sentinel-2, GHG-sat, etc). The observations are useful for the targeted monitoring of large point source emissions. The approach was previously experimented at oil and gas sites. Even though landfills are smaller sources in terms of emission strength compared to oil and gas sites, the feasibility of using a similar methodology on landfills has also been explored in a recent study, where strongly emitting landfills were detected in Buenos Aires.

6 References

- Chen, Tze-Ming, Janaki Gokhale, Scott Shofer, and Ware G Kushner. 2007. "Outdoor Air Pollution: Nitrogen Dioxide, Sulfur Dioxide, and Carbon Monoxide Health Effects." *The American Journal of the Medical Sciences* 333 (4): 249–56. <https://doi.org/10.1097/MAJ.0b013e31803b900f>.
- Crippa, M, D Guizzardi, M Muntean, E Schaaf, F Dentener, J A van Aardenne, S Monni, et al. 2018. "Gridded Emissions of Air Pollutants for the Period 1970--2012 within EDGAR v4.3.2." *Earth System Science Data* 10 (4): 1987–2013. <https://doi.org/10.5194/essd-10-1987-2018>.
- Gorroño, J, D J Varon, I Irakulis-Loitxate, and L Guanter. 2023. "Understanding the Potential of Sentinel-2 for Monitoring Methane Point Emissions." *Atmospheric Measurement Techniques* 16 (1): 89–107. <https://doi.org/10.5194/amt-16-89-2023>.
- Kaiser, J W, A Heil, M O Andreae, A Benedetti, N Chubarova, L Jones, J.-J. Morcrette, et al. 2012. "Biomass Burning Emissions Estimated with a Global Fire Assimilation System Based on Observed Fire Radiative Power." *Biogeosciences* 9 (1): 527–54. <https://doi.org/10.5194/bg-9-527-2012>.
- Maasakkers, Joannes D, Daniel J Varon, Aldis Elfarsdóttir, Jason McKeever, Dylan Jervis, Gourav Mahapatra, Sudhanshu Pandey, et al. 2024. "Using Satellites to Uncover Large Methane Emissions from Landfills." *Science Advances* 8 (32): eabn9683. <https://doi.org/10.1126/sciadv.abn9683>.
- Schuit, B J, J D Maasakkers, P Bijl, G Mahapatra, A.-W. van den Berg, S Pandey, A Lorente, et al. 2023. "Automated Detection and Monitoring of Methane Super-Emitters Using Satellite Data." *Atmospheric Chemistry and Physics* 23 (16): 9071–98. <https://doi.org/10.5194/acp-23-9071-2023>.
- Wiedinmyer, C, Y Kimura, E C McDonald-Buller, L K Emmons, R R Buchholz, W Tang, K Seto, et al. 2023. "The Fire Inventory from NCAR Version 2.5: An Updated Global Fire Emissions Model for Climate and Chemistry Applications." *Geoscientific Model Development* 16 (13): 3873–91. <https://doi.org/10.5194/gmd-16-3873-2023>.
- Xue, Chaoyang, Gisèle Krysztofiak, Yangang Ren, Min Cai, Patrick Mercier, Frédéric Le Fur, Corinne Robin, et al. 2024. "A Study on Wildfire Impacts on Greenhouse Gas Emissions and Regional Air Quality in South of Orléans, France." *Journal of Environmental Sciences* 135: 521–33. <https://doi.org/https://doi.org/10.1016/j.jes.2022.08.032>.

Signature

TNO) Energy & Materials Transition) Utrecht, 11 April 2024

Sam van Goethem
Research manager

Bart Jansen
Project manager

Appendix A

Background: Emission of Air Pollution and Methane

Uruguay is located in the southeastern region of South America with lush forests. The country has an economy featuring an export-oriented agricultural sector, demonstrated by a lot of farmlands. It is also surrounded by farmlands, forests, and urban areas from neighboring countries. Therefore, we can monitor air quality under the impact of forest fires and landfills in this study, as they are among the major contributors to the release of air pollutants and greenhouse gases into the atmosphere in Uruguay.

SO₂ and NO₂ can have side effects on the environment (such as the death of trees and harm to wildlife), human health, and air quality. NO₂ exposure may increase the risk of respiratory tract infections through the pollutant's interaction with the immune system. SO₂ contributes to respiratory symptoms, especially in those with underlying pulmonary disease (Chen et al. 2007). Forest fires produce a variety of pollutants into the atmosphere that impact air quality, atmospheric chemistry, and climate. The primary emissions include carbon monoxide, nitrogen oxides, particulate matter, and volatile organic compounds, with sulfur dioxide (SO₂) and nitrogen dioxide (NO₂) being the primary culprits. In recent years, forest fires have shown an increase in frequency and intensity due to changing climatic conditions and human activities.

Methane (CH₄) is a potent greenhouse gas that is emitted from landfill sites as a byproduct of the decomposition of organic waste. Methane can be emitted from landfills for many years after the waste has been deposited. Methane contributes to global warming both directly and indirectly through the release of carbon dioxide. In addition, methane reacts with hydroxyl radicals (OH), which clean many pollutants from the air, so increased methane reduces the amount of air pollutants removed by OH. Lastly, methane leads to the formation of ozone, which is also a greenhouse gas and causes negative impacts on plants, animals, and humans.

Prevention and mitigation efforts are necessary to minimize the impact of NO₂, SO₂, and CH₄ emissions. Elevated concentrations can serve as indicators of active or developing forest fires and landfill emissions. Knowing the distribution of elevated levels of these pollutants can allow for early interventions for regions located downwind of fires to prepare for potential air quality degradations and offer timely advisories to reduce health risks and protect the environment.

Appendix B

The CAMS Satellite Operator

The CAMS Satellite Operator (CSO) is a tool developed at TNO and implemented to facilitate the assimilation of Sentinel-5P observations. The tool consists of two entities:

- › a pre-processor to download, select, and convert satellite observations into a common format, accompanied by a post-processing tool to aggregate and visualize the data;
- › and a source code that could be included in regional air quality modelling and assimilation systems, and that can read the files created by the pre-processor, and simulate the observations using model variables.

B.1 Downloading observations

The first task that was performed by the pre-processor was to download satellite observation data from online archives. Given a time range and keywords that identify a particular data set, the scripts first created a list of orbit numbers that each Sentinel-5P image uniquely has. For NO₂ and SO₂, Level 2 datasets distributed by the official Sentinel mission were used (Product User Information and Algorithm Theoretical Basis Document can be found at <https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-5p/products-algorithms>). The datasets are also stored on NASA GES DISC. Subsequently, a list of HTTPS links was created to access NASA GES DISC (https://tropomi.gesdisc.eosdis.nasa.gov/data/S5P_TROPOMI_Level2/) for downloading. For CH₄, the Level 2 product from the Netherlands Institute for Space Research (SRON) was used due to the significantly improved data quality of the bias-corrected product (Algorithm Theoretical Basis Document <https://earth.sron.nl/wp-content/uploads/2023/12/SRON-ESA-S5L2PP-ATBD-001.pdf>). The Level 2 methane retrievals were downloaded from the SRON FTP server (https://ftp.sron.nl/open-access-data-2/TROPOMI/tropomi/CH4/19_446/). It should be noted that Level 2 data are already pre-processed and contain vertical column density for SO₂ and NO₂ and total column-average dry-air mole fraction for CH₄.

B.2 Conversion to CSO format

The Sentinel-5P observation files downloaded are huge in file size. The content includes various intermediate retrieval variables and diagnostics, some of which are not necessary for the simulation of observations by an air quality model. In addition, the files contain all pixels for a complete orbit (daytime part), while for in this project, only a subset over South America is needed. The CSO pre-processor therefore applies a conversion that selects only the required variables and pixels and saves the result in a CSO-specific format.

The conversion step has the following properties. The user can specify pixel selection criteria. One important selection criterion is the spatial domain in longitude and latitude coordinates. In addition, a selection on retrieval quality might be useful to further reduce the data volume. A minimum set of variables should be included in a data extract to simulate the satellite observations from model fields. These include:

- › Pixel footprints as corners in longitude/latitude coordinates.
- › Retrieval value(s), as column (single value) or profile.
- › If applicable, vertical layer definition of retrieval profile, in terms of air pressures at layer interfaces.
- › If available, a priori retrieval profile.
- › Averaging kernel profile(s).
- › Vertical layer definition used by the kernel (referred to as the a priori layers).
- › Retrieval error variance (for columns) or co-variance (for profiles).
- › Extra variables that could be useful for model validation and pixel selection during assimilation such as:
 - Quality flags;
 - Cloud properties;
 - Solar zenith angles.

Appendix C

Filtering criteria of NO₂, SO₂ and CH₄ from Sentinel-5P observations

NO₂

Based on the Product User Guide and the evaluation by the models, the following recommendations are made on using the S5p/NO₂ observations.

- › The product has a quality flag (variable 'qa_value') with a number in [0,1] to define the expected accuracy of a retrieval. For comparison with model simulations, it is advised that the minimum value should be 0.75, which excludes all (partly) clouded pixels and other problematic retrievals. Evaluation of the product showed that for lower thresholds (between 0.50 and 0.75), some averaging kernel profiles contained rather high values; the minimum value of 0.75 removed these.
- › The S5p/NO₂ product contains a special cloud variable dedicated to the wavelengths used by the retrieval, named 'cloud_fraction_crb_nitrogendioxide_window'. Selection of quality values above 0.75 re-moves all pixels that are (partly) clouded; alternatively, this cloud fraction could be used to exclude (partly) cloudy pixels.

SO₂

The S5p/SO₂ retrievals have been evaluated for the period of study (2018 Jun-Aug). This has led to the following recommendations for pixel selection.

- › The pixels at the edge of the swath are more noisy; following (Theys et al., 2019), only ground pixels 25-425 out of 1-450 are used.
- › The quality value should be at least 0.54.
- › Only pixels for solar-zenith angles below 70 degrees should be included.
- › Pixels should be cloud-free, and a cloud fraction threshold of a maximum of 0.2 is used.
- › The product contains a sulfur dioxide detection flag with values in the range 0 to 4; when values 1 to 3 are selected, only pixels are included near known sources such as volcanos and large power or industrial plants.

CH₄

For data use, it is sufficient to focus on the 'xCH₄' bias corrected product, the precision available in the data product (defined as the standard deviation of the retrieval noise, which describes the effect of the measurement noise on the retrieval), and the quality descriptor (qa_value). The qa_value indicates the status and quality of the retrieval output. To ensure that the highest quality data is used, only pixels that are classified with qa_value > 0.5 should be used. In case ocean and land, measurements need to be used separately, either the 'processing quality flag' or 'surface classification' mask should be used to select pixels with the 'sun glint warning' and 'water' flags.

Energy & Materials Transition

Princetonlaan 6
3584 CB Utrecht
www.tno.nl