

SOLFEO

ESA Contract No 4000127610/19/I-NS

Product User Guide

NH₃ emissions

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Author(s): Jieying Ding

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1 Introduction

1.1 Service description

Up-to-date and reliable emission inventories are essential for accurate air quality modelling and forecasting on various spatial scales. These inventories are also used by policy makers to evaluate the effectiveness of emission abatement measures, and to decide on future strategies. Here we use satellite observations of air constituents for deriving emissions. An advantage of these top-down emission estimates is the spatial and temporal consistency for all pollutants, a high temporal resolution, and the rapid availability.

Within the SOLFEO project emissions are derived for South America. The NH₃ emissions are derived with the DECSO inversion algorithm applied to IASI observations.

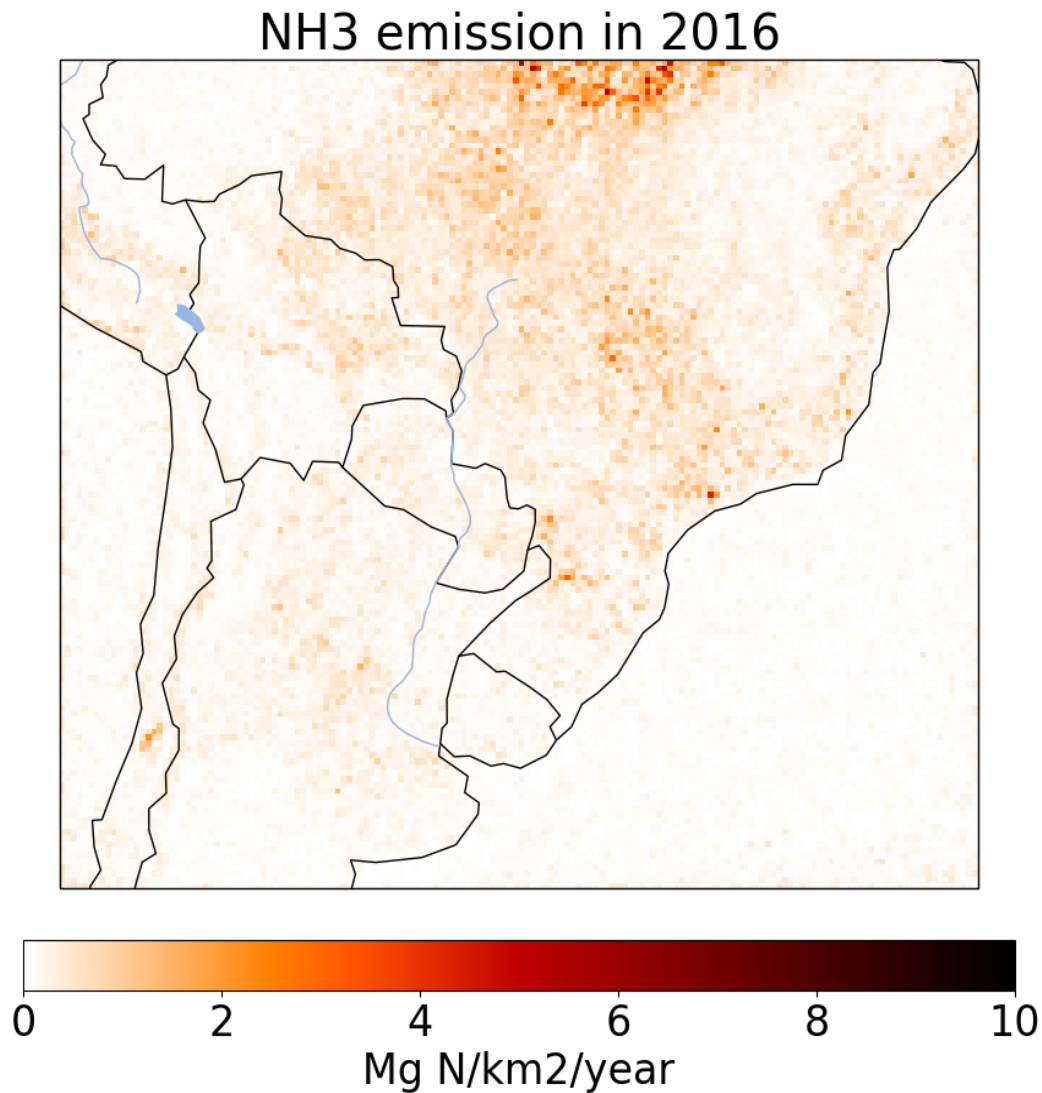


Figure 1. NH₃ emission for the year 2016 derived from the IASI observation from MetOp-A using the DECSO algorithm.

1.2 DECSO algorithm description

The DECSO algorithm [Mijling and Van der A, 2012] is specifically designed to use daily satellite observations of column concentrations for fast updates of emission estimates of short-lived atmospheric constituents on a mesoscopic scale ($0.25^\circ \times 0.25^\circ$). An extensive description of the algorithm can be found in the GlobEmission ATBD [2015].

We use the DECSO algorithm together with the regional chemistry-transport model CHIMERE on a 0.25° resolution, driven by operational meteorological forecast of the European Centre for Medium-Range Weather Forecasts (ECWMF). The model implementation is described in more detail by Ding et al. [2015]. We use NH₃ observations from the IASI instrument aboard the

MetOp-A satellite launched in October 2006. IASI is an infrared Fourier transform spectrometer, which circles in a polar Sun-synchronous orbit and operates in a nadir viewing mode with overpass times at 9:30 and 21:30 local solar time when it crosses over the Equator. IASI has an observational swath width of over 2000 km and a square field of view composed of four circular footprint of 12 km each at nadir, distorted to ellipse-shaped pixels off-nadir. We use the ANNI NH3 v2.1 reanalysis retrieval product from Van Damme et al. (2017). This product uses a neural network to link the hyperspectral range index (HRI) with a set of parameters, representing the atmospheric state, to derive the total NH₃ columns. The reanalysis dataset has small discontinuities by using the meteorological parameters from the ERA-Interim reanalysis and cloud coverage from EUMETSAT in near-real time. The dataset is downloaded from the Aeris data infrastructure (<https://iasi.aeris-data.fr/nh3/>). To use the data, we filter out the data lower than 4.8×10^{15} molecule/cm² due to the detection limit of IASI (2ppb, which is about 4.8×10^{15} molecule/cm²) (Dammers et al., 2019).

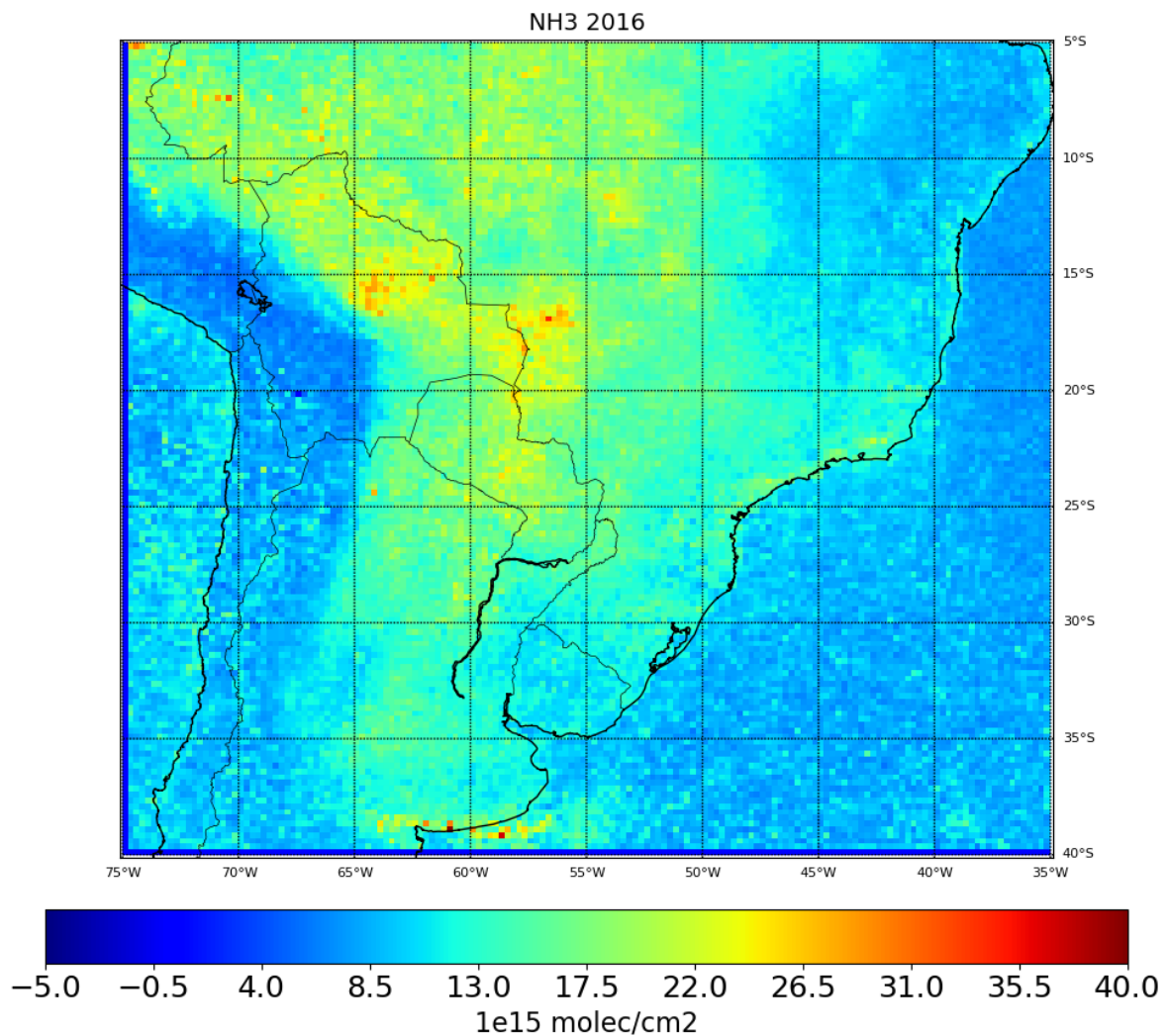


Figure 2 Averaged tropospheric NH₃ columns as observed by the IASI instrument aboard MetOp-A in 2016.

2 Product Specifications

2.1 Product description

Table 1. Output product description for emission inventory.

| | |
|------------------------|---|
| Product Type | Emission inventory. Air pollutants included: NH ₃ |
| Spatial Resolution | 0.25 degrees |
| Temporal Range | January 2016 – December 2016 |
| Temporal Resolution | Monthly averaged |
| Estimated accuracy | 42% |
| Spatial Coverage | Domain: 40-5° S, 75-36° W |
| Format and Size | Format: netCDF Size: approximately 1.6 MB per file |
| Satellite data sources | IASI-MetOp-A |

- The NH₃ (ammonia) emissions based on IASI for South America can be found at http://www.globemission.eu/region_samerica/datapage_nh3.php

2.2 Data structure

In table 2 the data structures of the SOLFEO NH₃ emission data is presented. In principle, the meta data description as well as the variables describe the data set in it full extend. The meta data include the data origin, comments, and domain description. As such the data products are compliant with GEOSS recommendations ensuring easy access to the data.

Table.2 Data structure for regional DECSO emission data in South America.

| Attribute | Meta Data Description |
|-----------------|-----------------------------------|
| X1: Description | Product description |
| X2: Author | name of creator |
| X3: Institution | name of institute |
| X4: Domain | Region with available data |
| X5: Year | Time period of emission inventory |

| | |
|------------------------|--|
| X6: History | Date of creation |
| X7: grid_westb | west bound of regular grid |
| X8: grid_westb_unit | units of west bound of regular grid |
| X9: grid_eastb | east bound of regular grid |
| X10: grid_eastb_unit | units of east bound of regular grid |
| X11: grid_lon_res | longitudinal resolution of regular grid |
| X12: grid_lon_res_unit | units of longitudinal resolution of regular grid |
| X13: grid_dlon | longitudinal spacing of regular grid |
| X14: grid_dlon_unit | units of longitudinal spacing of regular grid |
| X15: grid_south | south bound of regular grid |
| X16: grid_southb_unit | units of south bound of regular grid |
| X17: grid_northb | north bound of regular grid |
| X18: grid_northb_unit | units of north bound of regular grid |
| X19: grid_lat_res | latitudinal resolution of regular grid |
| X20: grid_lat_res_unit | units of latitudinal resolution of regular grid |
| X21: grid_dlat | latitudinal spacing of regular grid |
| X22: grid_dlat_unit | units of latitudinal spacing of regular grid |
| Variable | Description + unit |
| V1: time | Time in days since the beginning of the year |
| V2: lat | cell latitudes in regular grid (cell centers) [degrees_north] |
| V3: lon | cell longitudes in regular grid (cell centers) [degrees_east] |
| V4: NH3 | ammonia emission from source [10^{15} molecules/cm ² /h] |
| V5: NH3_alt | ammonia emission from source [Gg N/cell/month] |
| V6: area | cell area in regular grid [km ²] |
| Dimensions | Definition |
| time | Dimension of the time variable |
| lat | Dimension of the variable lat |
| lon | Dimension of the variable lon |

3 Data quality and known issues

3.1 High altitudes

The CTM used in DECSO is modeling till a pressure level of about 500 hPa. For very high mountain ranges this can lead to too small model layers with unrealistic local model results. This can lead to unrealistic emissions over the Andes. Therefore, all data for grid cells with an average altitude above 3500 m has been removed. Figure 3 shows the altitude in the region of the emissions.

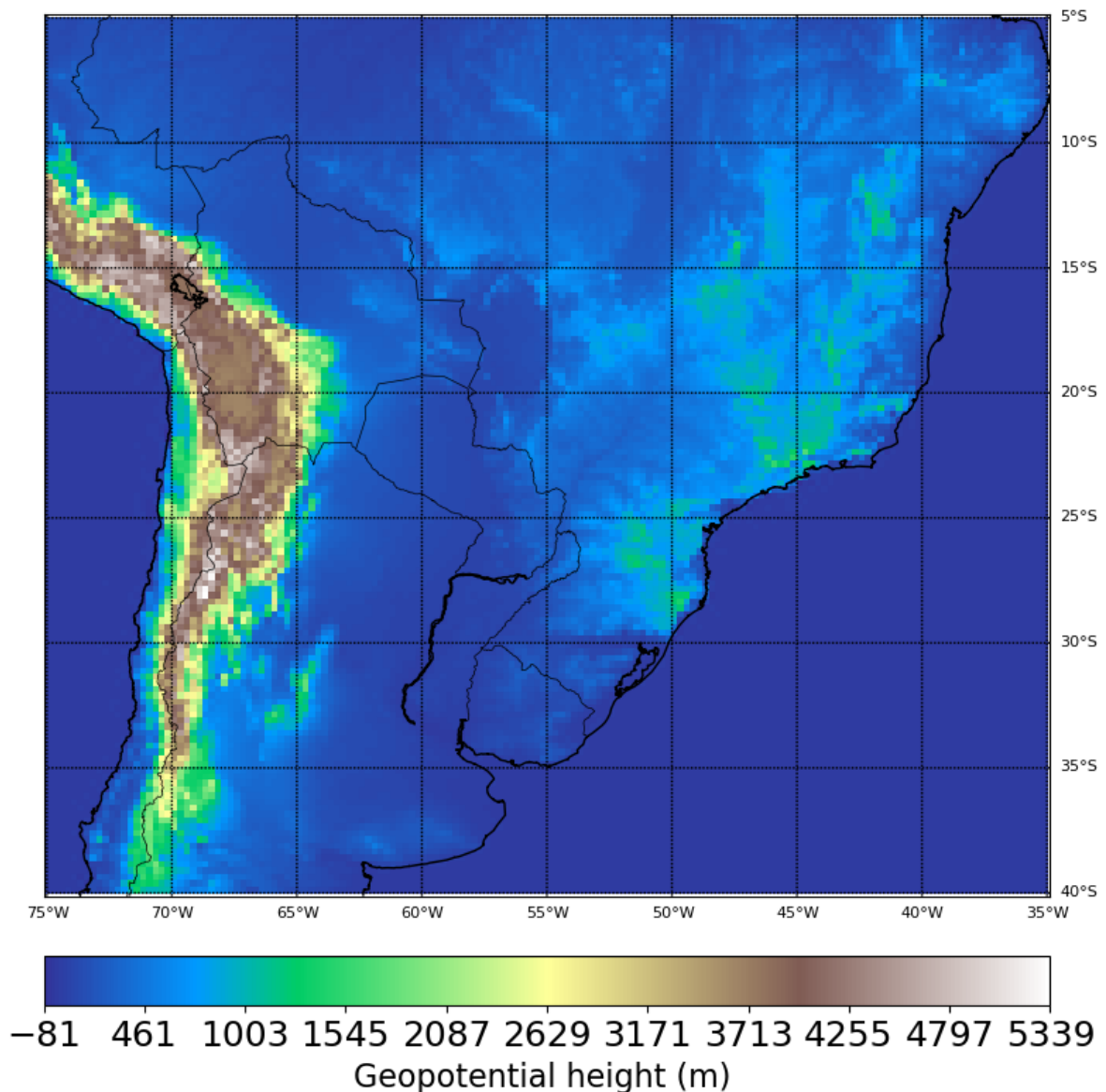


Figure 3 Geopotential height (m) in the region for which the emissions are provided.

3.2 IASI NH₃ validation

We use the NH₃ retrieval product of the version ANNI-NH3-v2.1R-I. The product combines the calculation of the dimensionless spectral index (HRI) with a neural network to calculate the total columns of NH₃. Dammers et al. (2019) and Van Damme et al. (2018) estimated NH₃ emissions from point sources using the same NH₃ retrieval product. The previous versions of the NH₃ product were validated by Dammers et al. (2016) and were found to have a low bias of about 40% and with better performance for the regions with high concentrations. Van Damme et al. (2017) stated that the ANNI NH₃ v2.1 reanalysis retrieval product used for NH₃ emission estimates is self-consistent in time and is expected to be highly suitable to study long-term trends.

References:

Dammers, E., Palm, M., Van Damme, M., Vigouroux, C., Smale, D., Conway, S., Toon, G. C., Jones, N., Nussbaumer, E., Warneke, T., Petri, C., Clarisse, L., Clerbaux, C., Hermans, C., Lutsch, E., Strong, K., Hannigan, J. W., Nakajima, H., Morino, I., Herrera, B., Stremme, W., Grutter, M., Schaap, M., Wichink Kruit, R. J., Notholt, J., Coheur, P.-F., and Erisman, J. W.: *An evaluation of IASI-NH₃ with ground-based Fourier transform infrared spectroscopy measurements*, *Atmos. Chem. Phys.*, 16, 10351–10368, <https://doi.org/10.5194/acp-16-10351-2016>, 2016.

Dammers, E., McLinden, C. A., Griffin, D., Shephard, M. W., Van Der Graaf, S., Lutsch, E., et al. (2019). *NH₃ emissions from large point sources derived from CrIS and IASI satellite observations*. *Atmos. Chem. Phys.*, 19(19), 12261-12293. doi:10.5194/acp-19-12261-2019

Van Damme, M., Whitburn, S., Clarisse, L., Clerbaux, C., Hurtmans, D., and Coheur, P.-F.: *Version 2 of the IASI NH₃ neural network retrieval algorithm: near-real-time and reanalysed datasets*, *Atmos. Meas. Tech.*, 10, 4905–4914, <https://doi.org/10.5194/amt-10-4905-2017>, 2017.

Van Damme, M., Clarisse, L., Whitburn, S., Hadji-Lazaro, J., Hurtmans, D., Clerbaux, C., & Coheur, P.-F. (2018). *Industrial and agricultural ammonia point sources exposed*. *Nature*, 564(7734), 99-103. doi:10.1038/s41586-018-0747-1

3.3 Comparison to HTAP

We use the HTAP (Hemispheric Transport Atmospheric Pollution) emission inventory version 2 in 2010 as our initial emissions to run the CTM. The spatial resolution of HTAP is 0.1° × 0.1°. HTAP uses nationally reported emissions combined with regional scientific inventories in the format of sector-specific grid maps. The database consists of a combination of gridded regional emission inventories such as the Model Inter-Comparison Study (MICS) for Asia, Environmental Protection Agency (EPA) for the US and Canada, and the Netherlands Organisation for Applied Scientific Research – Monitoring Atmospheric Composition and Climate (TNO-MACC) II database for Europe. The grid maps are complemented with EDGARv4.3 data for those regions where data are absent.

Figure 4 presents the monthly NH₃ emissions from HTAP in 2010. We see NH₃ emissions slightly increase or decrease with the same spatial distribution from month to month. Since the

lifetime of NH_3 is very short, about a few hours, we expect the NH_3 emission distribution to be similar to the concentration. The monthly NH_3 column concentrations observed by IASI show different monthly distributions (Figure 5). We see a very strong seasonal variation on NH_3 column concentrations in the region. NH_3 column concentrations start to increase in the center of the domain in August. The high NH_3 concentrations are due to biomass burning emissions (van Damme et al., 2018). Figure 6 shows the NH_3 monthly emissions derived from satellite observations. We see a clear seasonal cycle from the figure.

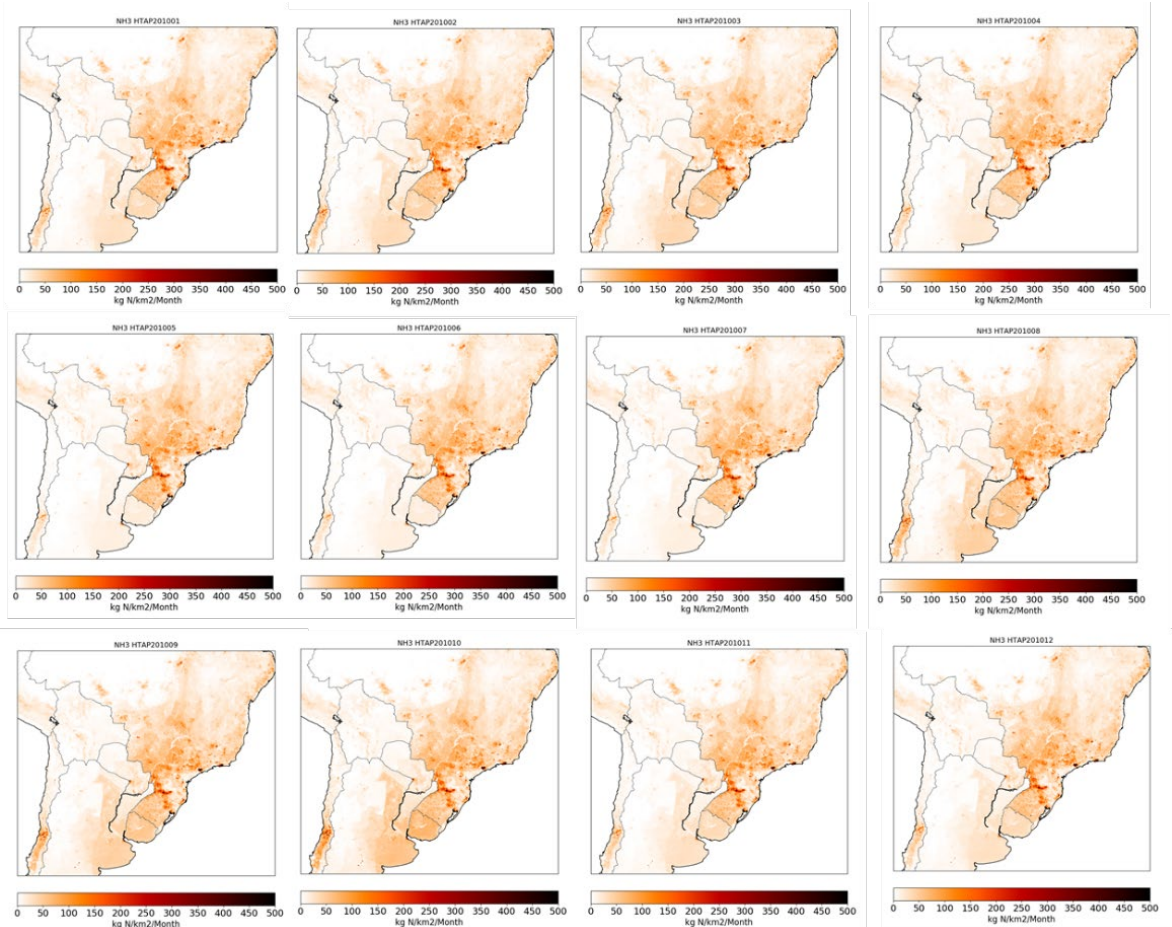


Figure 4. Monthly NH_3 emissions from HTAP 2010. Data are downloaded from https://edgar.jrc.ec.europa.eu/htap_v2/.

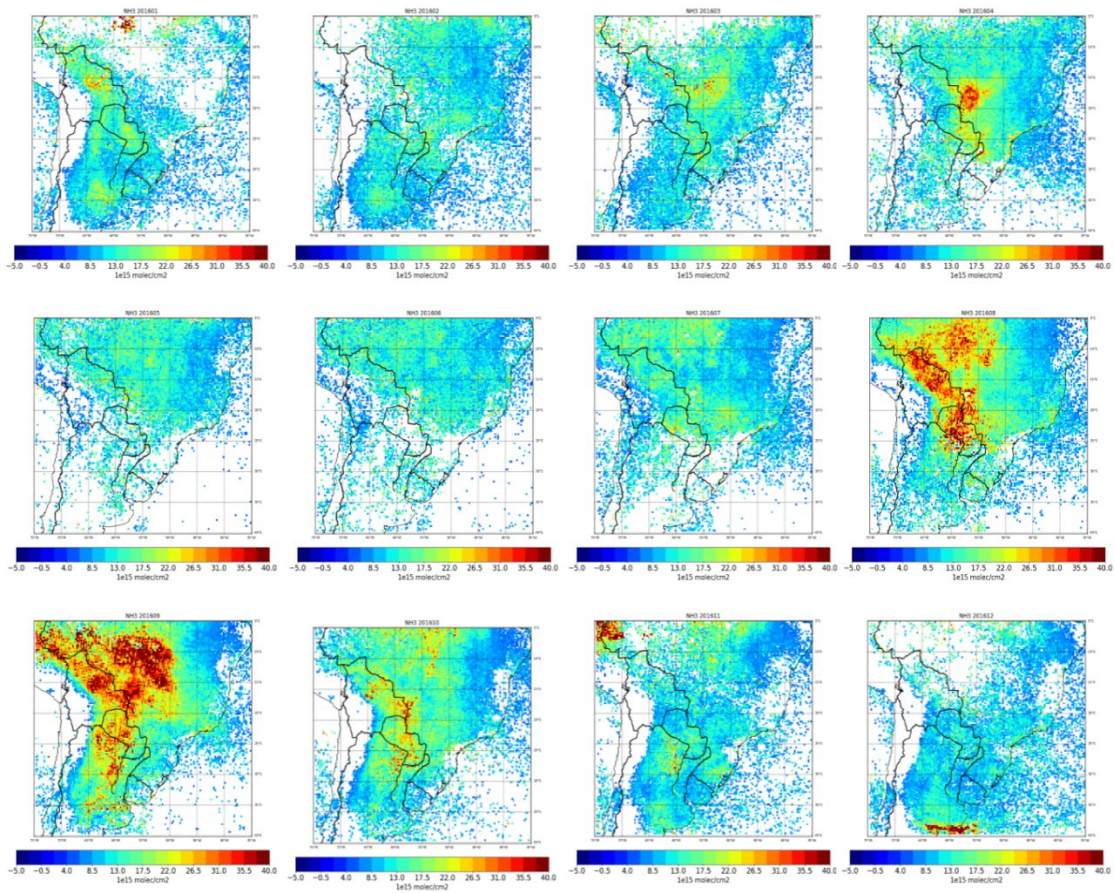


Figure 5. Monthly tropospheric NH₃ columns in 2016 as observed by the IASI instrument aboard MetOp-A.

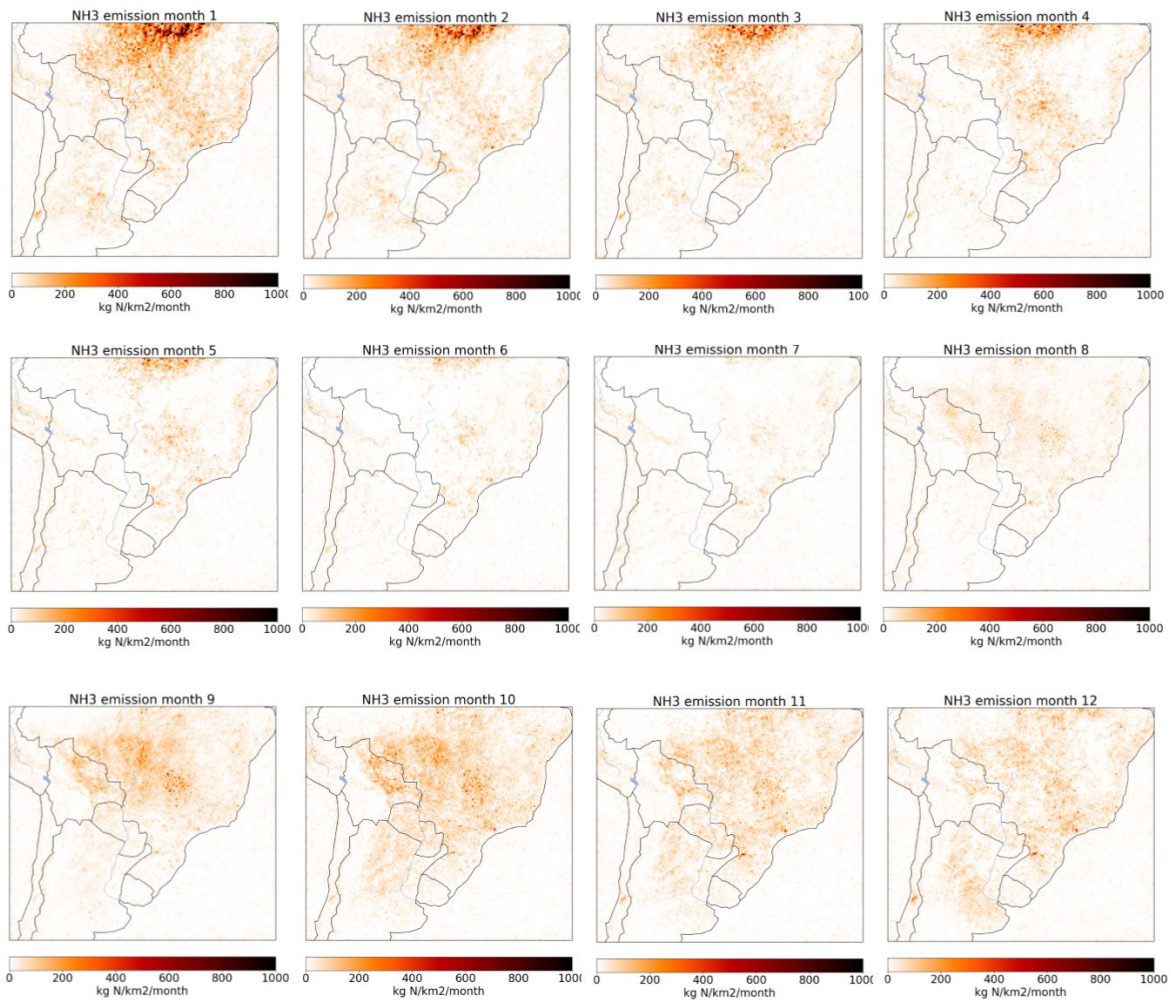


Figure 6. Monthly NH₃ emissions in 2016 derived with DECSO from IASI observations on MetOp-A.

3.4 Comparison to an Argentinian bottom-up inventory

We have compared the DECSO emissions to an Argentinian bottom-up emission inventory recently published in Puliafito et al.(2020). The bottom-up inventory contains emission for the year 2014 and 2016. We have resampled the 2016 NH₃ emissions to the same grid as DECSO for comparison. Figure 7 shows the comparison between the annual bottom-up and the annual averaged NH₃ emissions of DECSO. The bottom-up inventory of Argentina shows that NH₃ emissions are mainly distributed in the east part of Argentina (see figure 7). Two strong point sources are shown in the city area of Buenos Aires and Concepción del Uruguay. However, these two strong points are not seen from satellite observations and also not found in the point source emission study from Dammers et al. (2019) and van Damme et al. (2018). Figure 7 shows that NH₃ emissions estimated with DECSO from IASI on MetOp-A are mainly distributed over cropland and herbaceous areas (see the land use map of Figure 8).

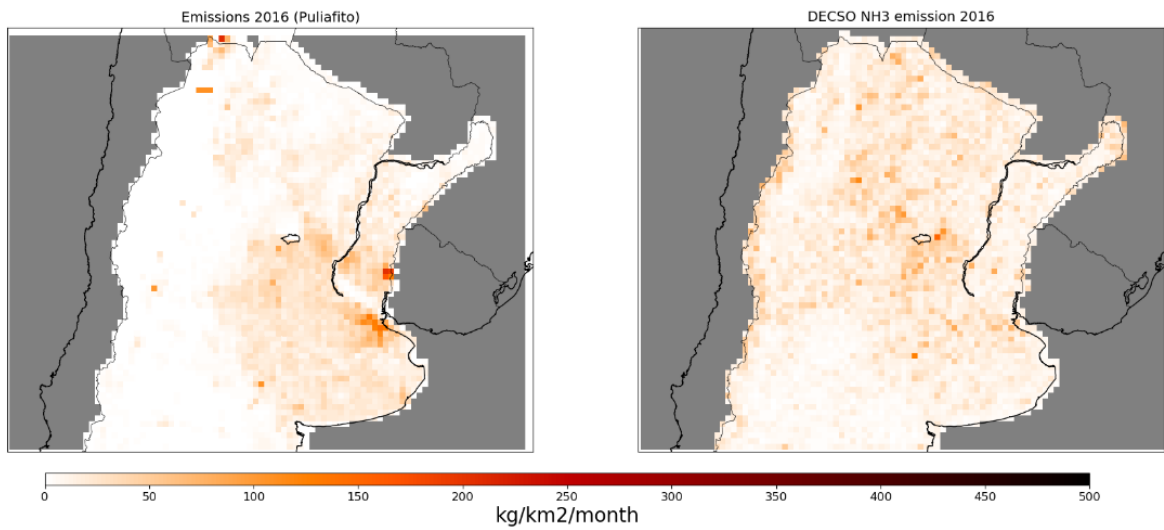


Figure 7 Comparison of the NH₃ emissions over Argentina from the bottom-up inventory in 2016 (left plot) and the DECSO emissions in 2016 (right plot).

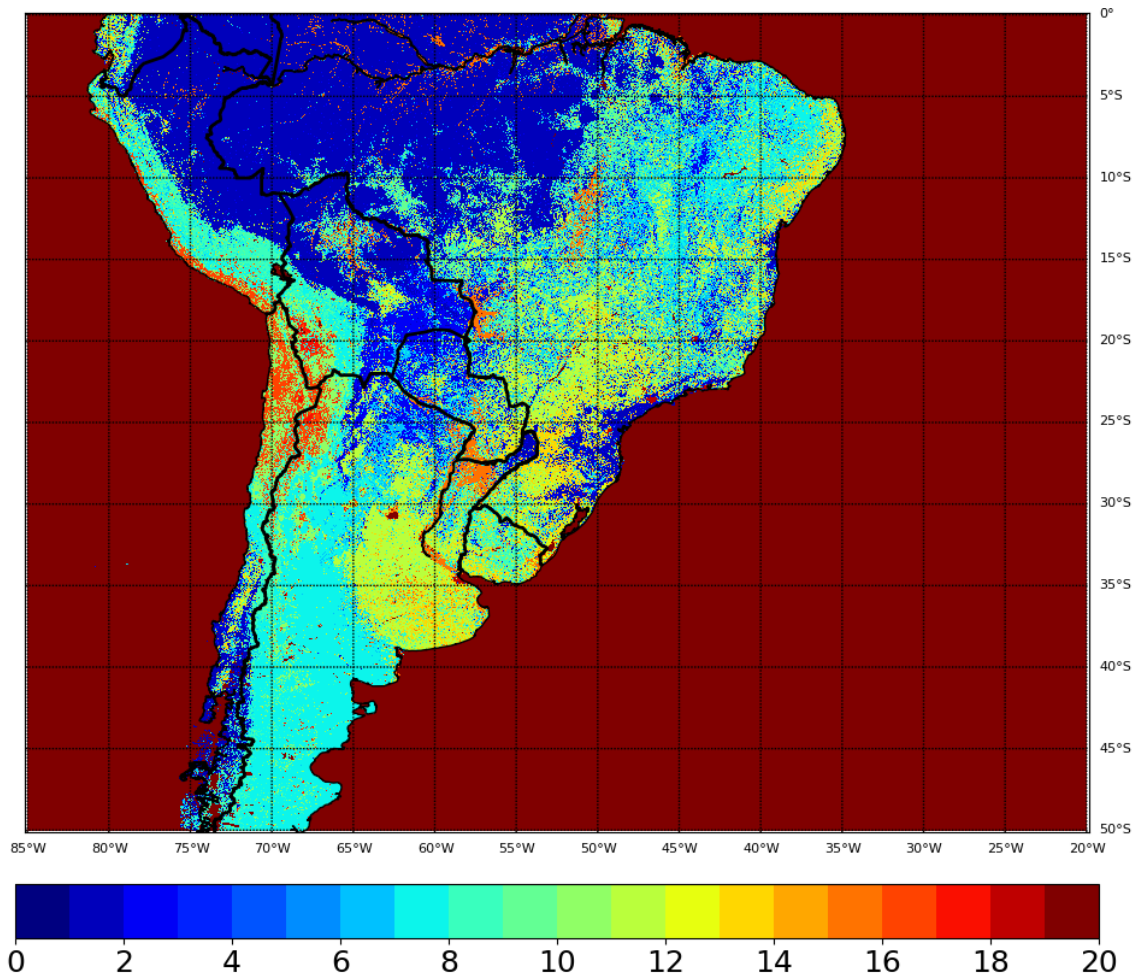


Figure 8. Landuse map in South America in 2013. The number represents different landuse categories. 1.Broadleaf Evergreen Forest; 2.Broadleaf Deciduous Forest; 3.Needleleaf Evergreen Forest; 4.Needleleaf Deciduous Forest; 5.Mixed Forest; 6.Tree Open; 7.Shrub; 8.Herbaceous; 9.Herbaceous with Sparse Tree/Shrub;

10.Sparse vegetation; 11.Cropland; 12.Paddy field; 13.Cropland / Other Vegetation Mosaic; 14.Mangrove; 15.Wetland; 16. Bare area, consolidated (gravel, rock); 17. Bare area, unconsolidated (sand); 18.Urban; 19. Snow / Ice; 20. Water bodies. The landuse dataset is the product version 3 from the Global Land Cover by National Mapping Organizations (GLCNMO). The data were prepared by using MODIS data with remote sensing technology. More information about the data can be found on <https://globalmaps.github.io/glcnm.html>

Reference:

S. E. Puliafito, T. Bolaño-Ortiz, L. Berná, R. P. Flores, High resolution inventory of atmospheric emissions from livestock production, agriculture, and biomass burning sectors of Argentina, Atm. Environment, 223, 117248, doi:10.1016/j.atmosenv.2019.117248, 2020.

4 Publications related to DECSO

Ding, J., R.J. van der A, B. Mijling, P.F. Levelt and N. Hao, NO_x emission estimates during the 2014 Youth Olympic Games in Nanjing, *Atm. Chem. Phys.*, 2015, 15, 9399-9412, doi:10.5194/acp-15-9399-2015.

Ding, J., Miyazaki, K., van der A, R.J., Mijling, B., Kurokawa, J., Cho, S., Janssens-Maenhout, G., Zhang, Q., Liu, F., and Levelt, P.F., Intercomparison of NO_x emission inventories over East Asia, *Atm. Chem. Phys.*, 2017, 17, 10125-10141, doi:doi.org/10.5194/acp-17-10125-2017.

Ding, J., R.J. van der A, B. Mijling and P.F. Levelt, Space-based NO_x emission estimates over remote regions improved in DECSO, *Atmospheric Measurement Techniques*, 2017, 10, 925-938, doi:10.5194/amt-10-925-2017.

Ding, J., van der A, R. J., Mijling, B., Jalkanen, J.-P., Johansson, L. and Levelt, P. F., Maritime NO_x emissions over Chinese seas derived from satellite observations. *Geophysical Research Letters*, 45. <https://doi.org/10.1002/2017GL076788>, 2018.

Mijling, B., R.J. van der A, K.F. Boersma, M. Van Roozendaal, I. De Smedt and H.M. Kelder, *Reduction of NO₂ detected from space during the 2008 Beijing Olympic Games*, *Geophys. Res. Lett.*, 2009, 36, doi:10.1029/2009GL038943.

Mijling, B. and R.J. van der A, Using daily satellite observations to estimate emissions of short-lived air pollutants on a mesoscopic scale. *J. Geophys. Res.* 117, D17, doi:10.1029/2012JD017817, 2012.

Mijling, B., R.J. van der A and Q. Zhang, Regional nitrogen oxides emission trends in East Asia observed from space. *Atmos. Chem. Phys.*, 13, 12003-12012, doi:10.5194/acp-13-12003-2013, 2013.

van der A, R. J., Mijling, B., Ding, J., Koukouli, M. E., Liu, F., Li, Q., Mao, H., and Theys, N., Cleaning up the air: Effectiveness of air quality policy for SO₂ and NO_x emissions in China, *Atm. Chem. Phys.*, 2017, 17, 1775-1789, doi:10.5194/acp-17-1775-2017.

van der A, R.J., de Laat, A.T.J., Ding, J., Eskes, H.J., Connecting the dots: NO_x emissions along a West Siberian natural gas pipeline, *npj Clim Atmos Sci* 3, 16, <https://doi.org/10.1038/s41612-020-0119-z>, 2020.