Ammonia observation and modeling simulation 2

IASI data and GEO-Chem model

2020.9

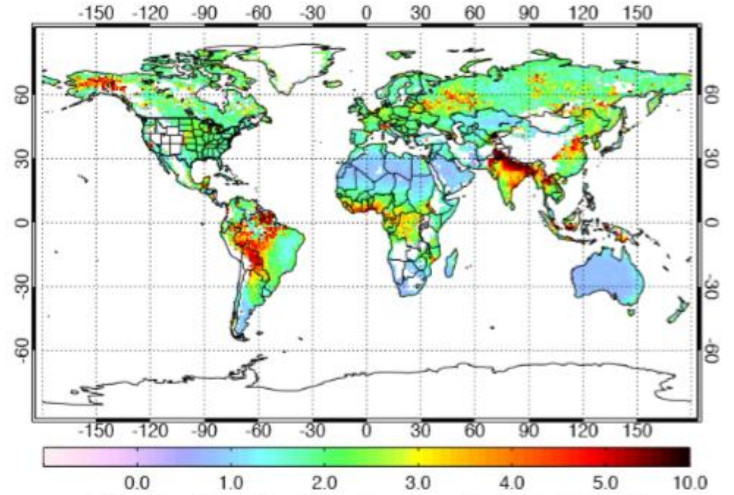
- Accomplished:
  - 1. literature: global ammonia distribution from IASI/AIRS
  - 2. literature: ammonia trend over the U.S.
  - 3. spatial distribution of seasonal mean and seasonal change over the SH, NH
  - 4. spatial distribution of seasonal trend and seasonal trend in the equivalent latitude
  - 5. PDF of the 2008-2016 and 2017 over seasonal day and night
  - 6. missing value count per month
- Ammonia Data:
  - IASI (2008-2017), 1°×1°, monthly, land area
    - Reanalyzed IASI/Metop-A (2008-2016) L3
    - Standard monthly IASI/Metop-A (2008-2017) L3
- Ongoing:
  - 1. learning <China and India lead in greening of the world through land-use management> (Chen et al., 2019)
  - 2. learning GEO-Chem manual and submitting the job

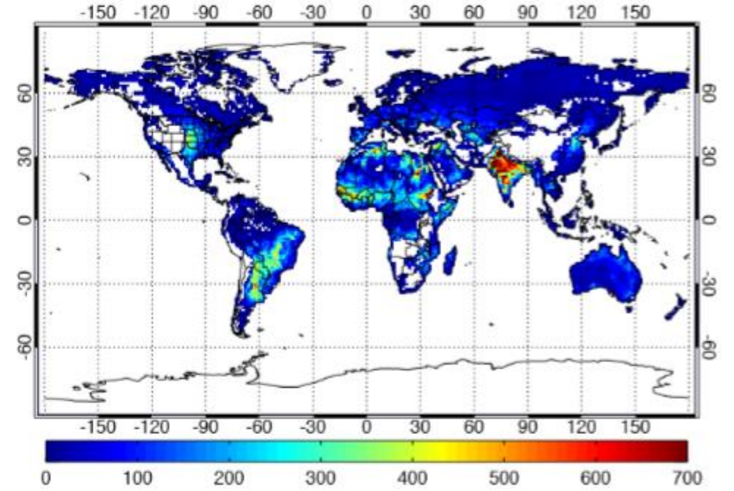
IASI

- Reanalyzed IASI/Metop-A (2008-2016) L3: processed using the standard daily IASI/Metop-A NH_3 L2 dataset
  - (1) account for complete temperature and humidity vertical profiles
  - (2) use third-party NH3 vertical profile information
  - (3) provide a full measurement uncertainty characterization
- Disclaimer:
  - The Eumetsat IASI PPF L2 data processing chain has been updated several times since IASI launch, inducing discontinuities in the retrieved NH3 time-series. A second dataset (ANNI-NH3-v3R-ERA5) which relies on ERA5 ECMWF meteorological input data, along with surface temperature retrieved from a dedicated network, rather than the operationally provided Eumetsat IASI Level 2 (L2) data used for the standard version is also available on AERIS Website. For inter-annual comparisons and trends analyses, only the reanalysed dataset should be used.

The global tropospheric ammonia distribution as seen in the 13-year AIRS measurement record

- present extensive and nearly continuous global ammonia measurements made by AIRS to identify and quantify major persistent and episodic sources as well as to characterize seasonality
- examine the 13-year period from 2002.9 through 2015.8 with a retrieval algorithm using an optimal estimation technique
- Global ammonia concentrations (NH3 VMRs at 918hPa)
  - The AIRS global: strong NH3 hotspots from biogenic and anthropogenic sources
  - the total occurrences of elevated concentrations (VMRs⩾1.0ppbv)

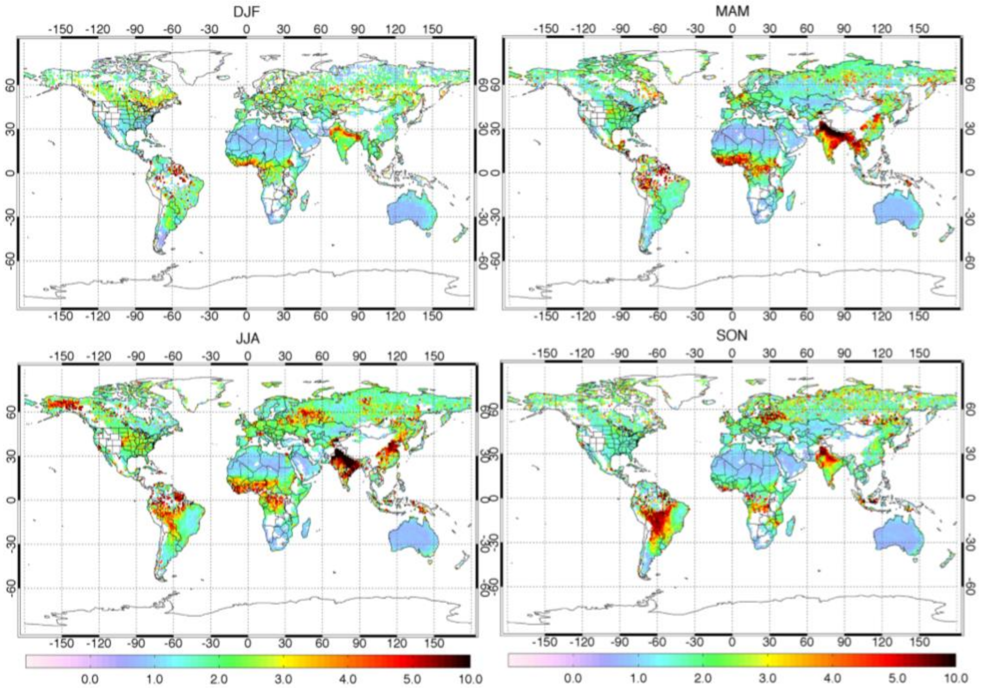


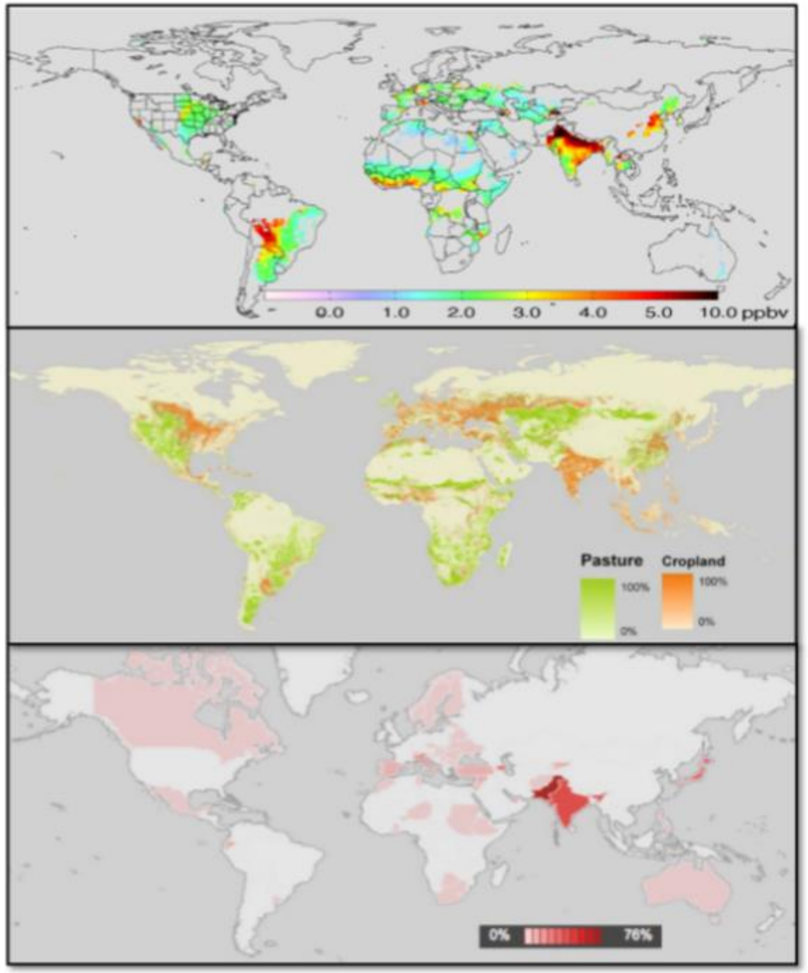


(Warner et al, 2016)

The global tropospheric ammonia distribution as seen in the 13-year AIRS measurement record

- Global ammonia concentrations (NH3 VMRs at 918hPa)
  - the collocated occurrences of elevated concentrations (⩾1.4ppbv) greater than 40 days
  - Pasture and Cropland Map: India, China, the middle US, Western Africa, eastern South America, and Europe
  - irrigated agricultural areas : Pakistan, India, northern Italy, and Azerbaijan
- Seasonal variability
  - Global averaged
    - biomass burning (BB)
    - Non-BB

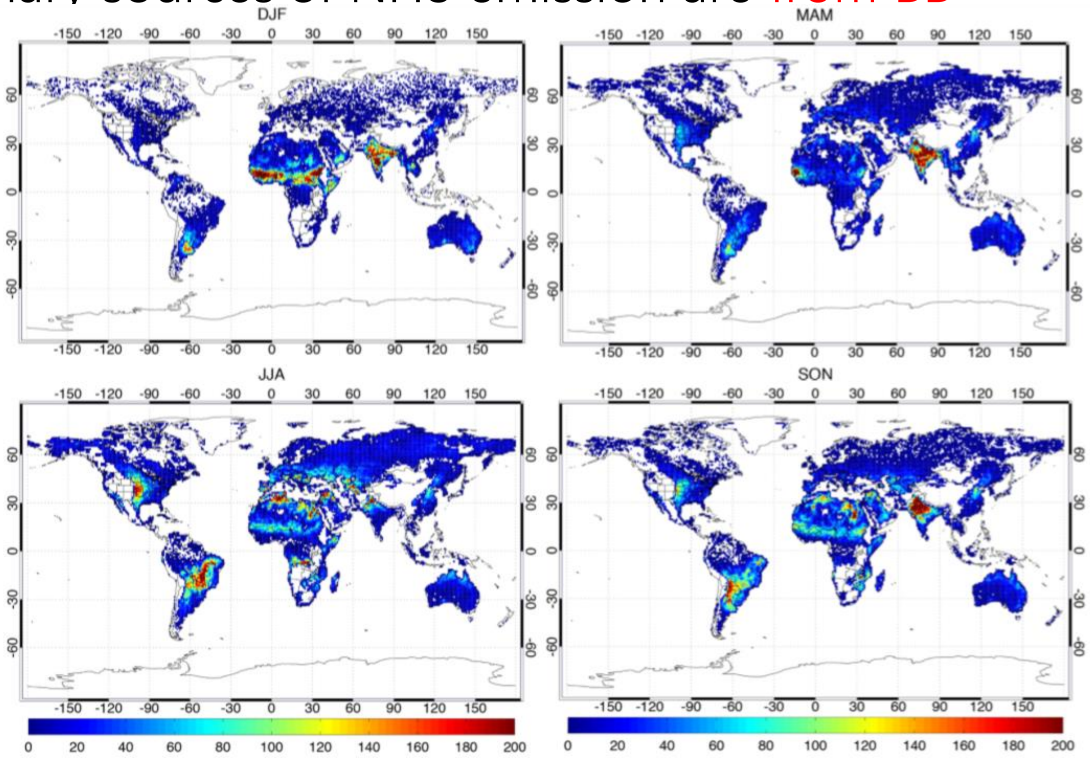


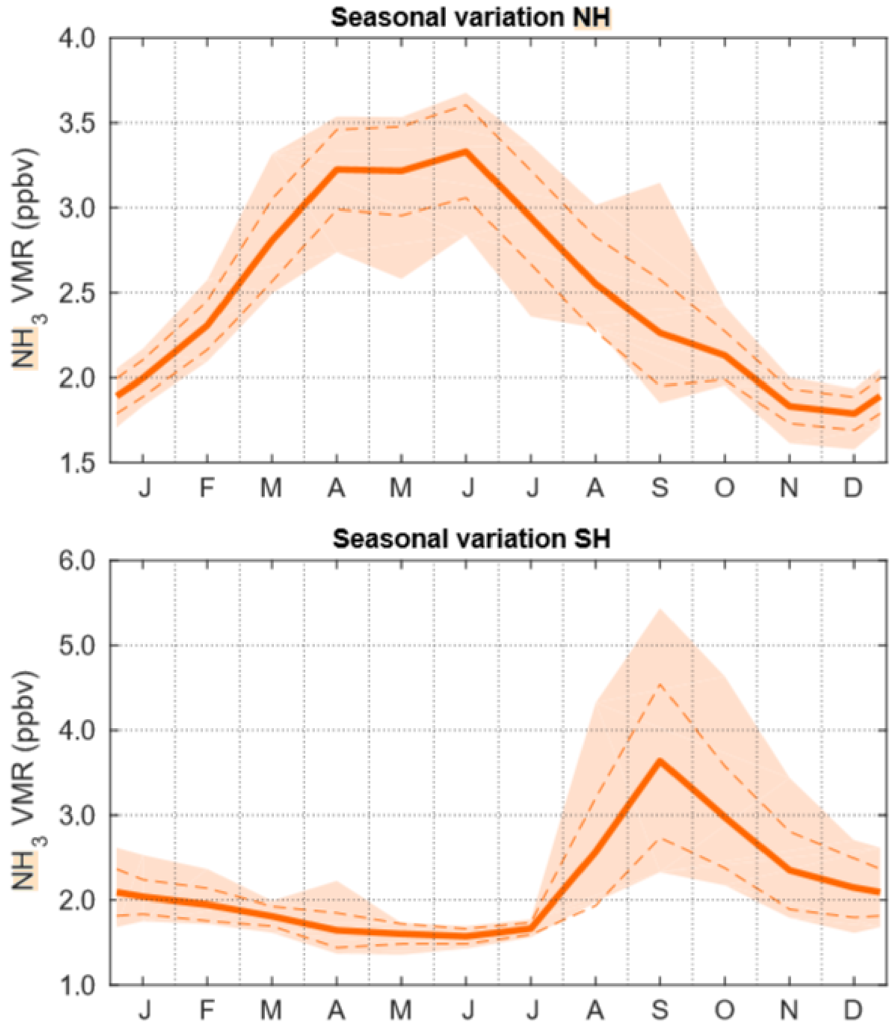


(Warner et al, 2016)

The global tropospheric ammonia distribution as seen in the 13-year AIRS measurement record

- Seasonal variability
  - occurrences of high concentrations (VMRs ⩾1ppbv): indicate NH3 from biomass burning (BB)
  - monthly mean variations
    - NH: Apr to June
    - SH: the primary sources of NH3 emission are from BB





(Warner et al, 2016)

Global distributions, time series and error characterization of atmospheric ammonia (NH3) from IASI satellite observations

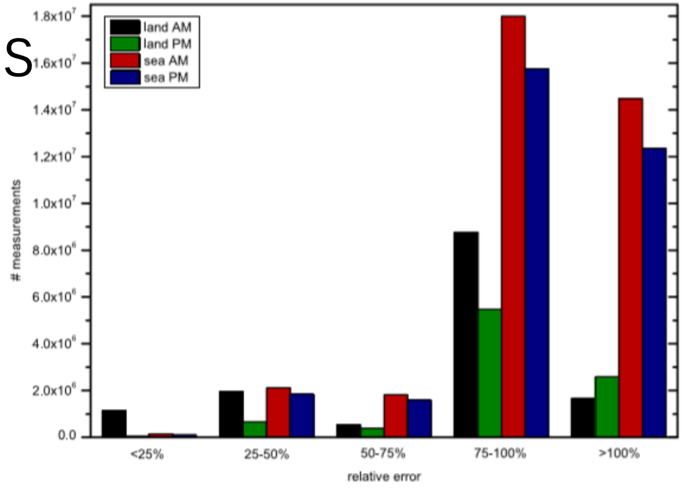
- describe an improved retrieval scheme of NH3 total columns from the measurements of the IASI
- show how to retrieve the NH3 total columns from IASI quasi-globally and twice daily above both land and sea without large computational resources and with an improved detection limit
- Provide spatial distributions from the five years data set and analyze at global and regional scales
- show the ability of this method to identify smaller emission sources than those previously reported, as well as transport patterns over the ocean
- examined in terms of seasonality and interannual variability separately for the Northern and Southern Hemispheres
- IASI
  - circles in a polar Sun-synchronous orbit
  - operates in a nadir-viewing mode with overpass times at 9:30 local solar time and 21:30 local solar time when it crosses over the Equator
  - 24 atmospheric species have been identified

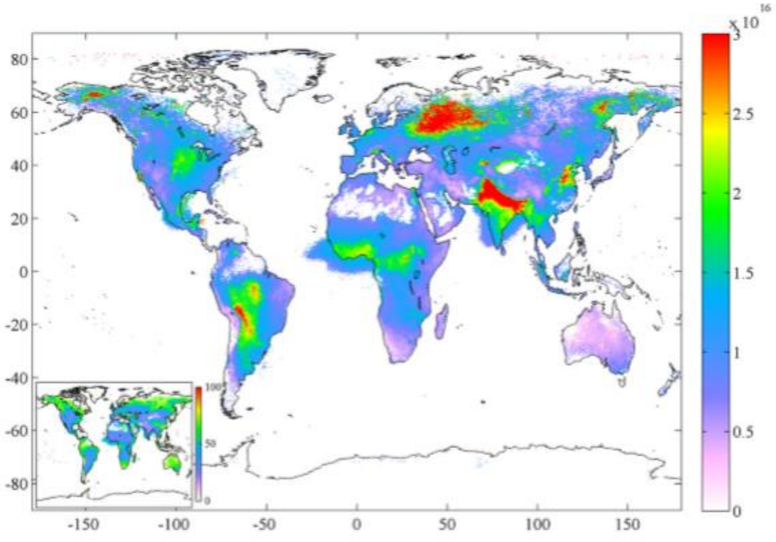
Global distributions, time series and error characterization of atmospheric ammonia (NH3) from IASI satellite observations

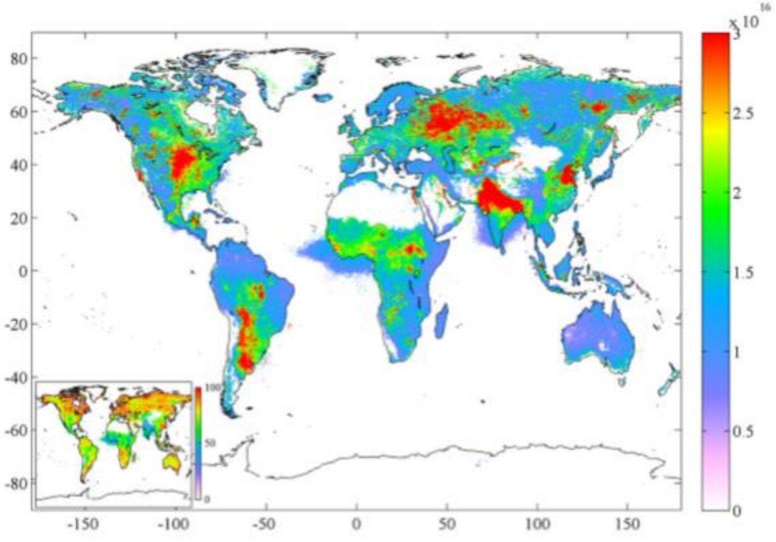
- Product evaluation
  - the relative error on the retrieved NH3 column (2007.11-2012.10): the majority of measurements have an error above 75%
- Global and regional distributions

$$\bar{x} = \frac{\sum w_i x_i}{\sum w_i}, \quad w_i = 1/\sigma^2 \text{ and } \sigma \text{ is the error } \quad \bar{\sigma} = \frac{\sum \frac{1}{\sigma_i}}{\sum \frac{1}{\sigma_i^2}}.$$

- Global and regional distributions
  - NH3 total column distribution: fire-related, agriculture



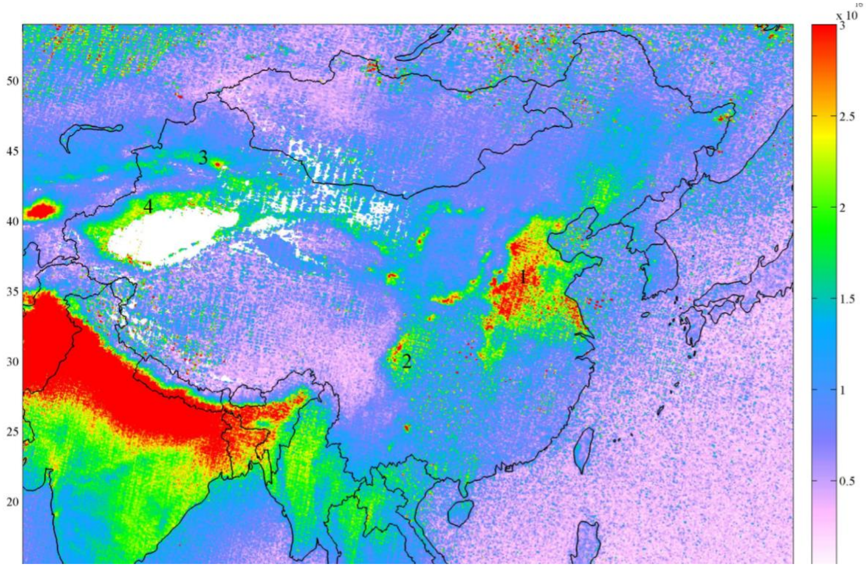


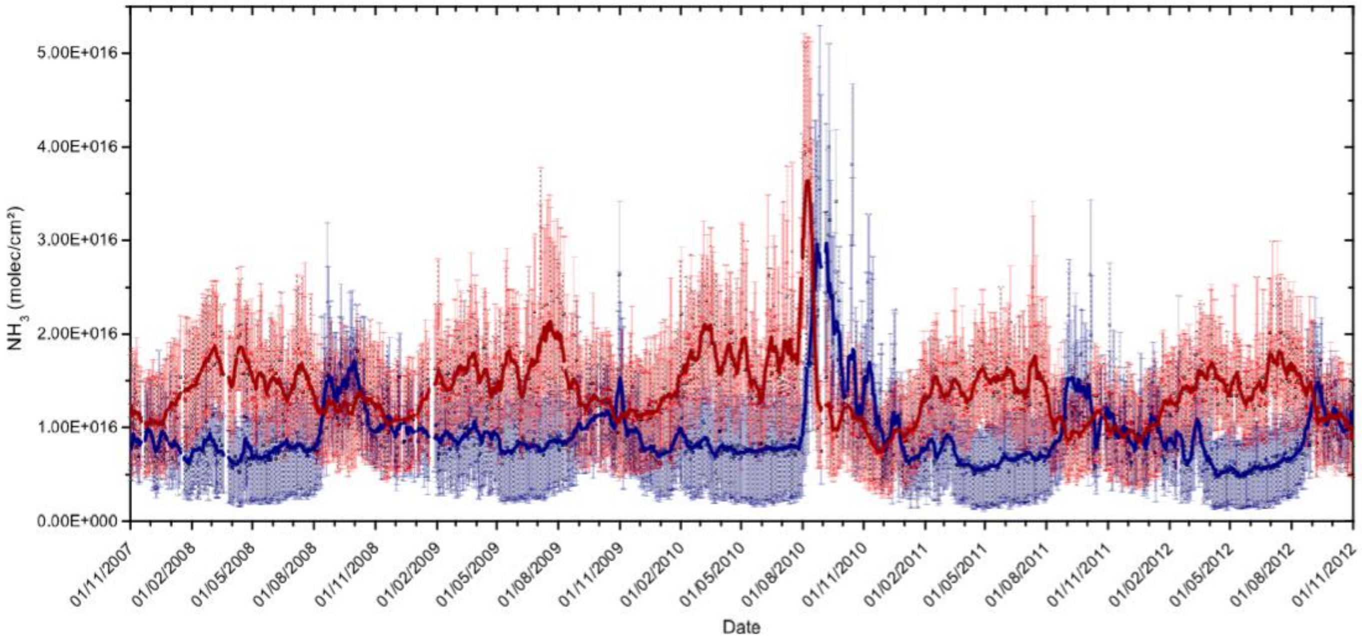


(Damme et al, 2016)

Global distributions, time series and error characterization of atmospheric ammonia (NH3) from IASI satellite observations

- Global and regional distributions
  - the regional NH3 distribution over eastern Asia
    - 1. larger column values in areas where there is intensive agriculture
    - 2. the emissions are mainly from livestock
- Temporal evolution
  - daily retrieved NH3 columns above: seasonal cycle

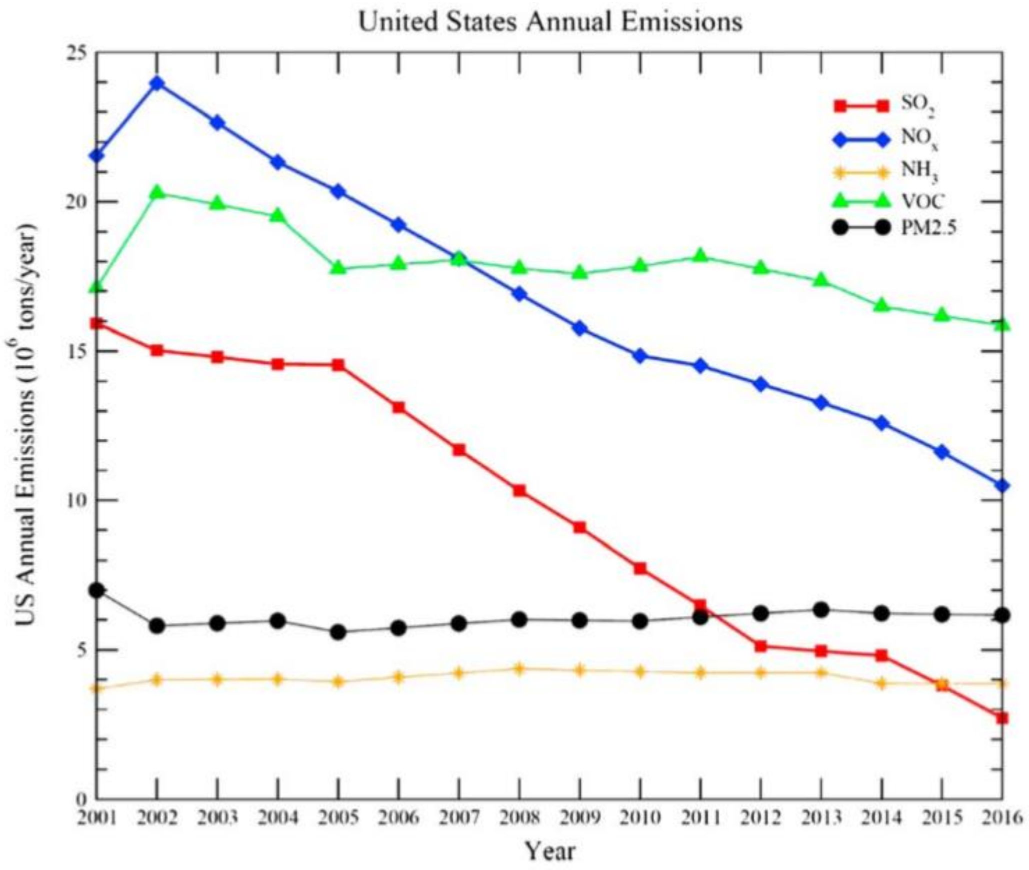




(Damme et al, 2016)

Long-Term Trend of Gaseous Ammonia Over the United States: Modeling and Comparison With Observations

- examine the long-term trend in [NH3] in the United States using a 3-D global tropospheric chemistry model——GEOS-Chem
- Compare the simulated [NH3] values and trends with those observed from a surface ammonia monitoring network
- determine the extent of the contribution of SO2 and NOx emission changes to the long-term [NH3] trends by considering various emission scenarios
- U.S. anthropogenic emissions:
  - a slight increase for NH3 emission from 2001 to 2008: fires, waste disposal, and municipal/commercial composting emmision
  - after 2008, NH3 emission decreased slightly: the decrease of miscellaneous emissions

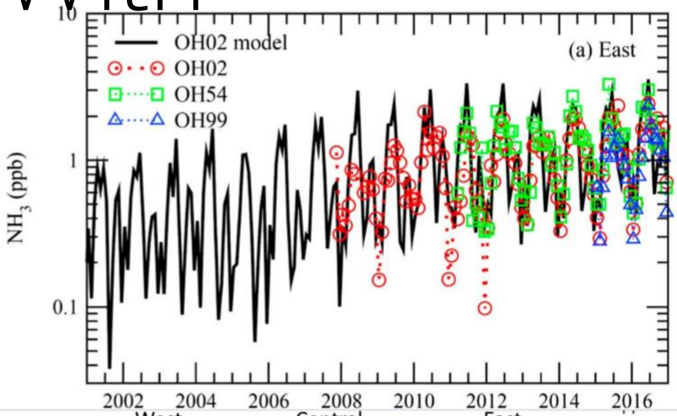


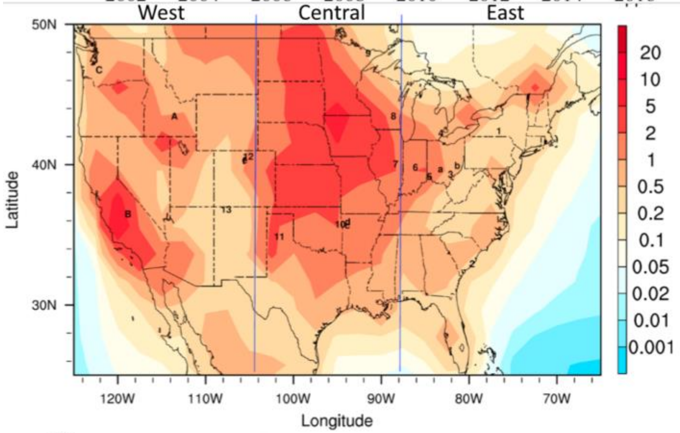
(Yu et al, 2018)

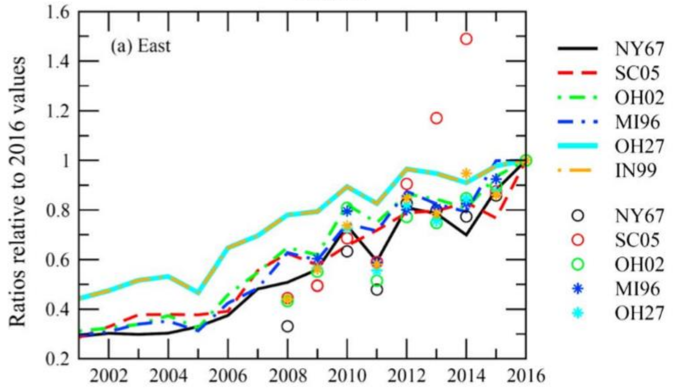
Long-Term Trend of Gaseous Ammonia Over the United States: Modeling and Comparison With Observations

- Spatial Distribution of [NH3] Over the United States
  - The average surface layer simulated:
    - regions with relatively higher ammonia surface concentrations tend to have more intensive agriculture activities
  - Modeled and observed sites long-term trend of ammonia in selected sites
    - the long-term trend seen in the model is valid
    - cautions against use of surface measurements as representative of regional concentrations
- Increasing Long-Term Trend of [NH3]
  - the linear trend of model simulated surface layer ammonia
    - the ammonia hotspots appear to show a less increasing or decreasing trend
  - Long-term trend of [NH3] in sites
    - The long-term increase is evident for most of the selected sites

(Yu et al, 2018)

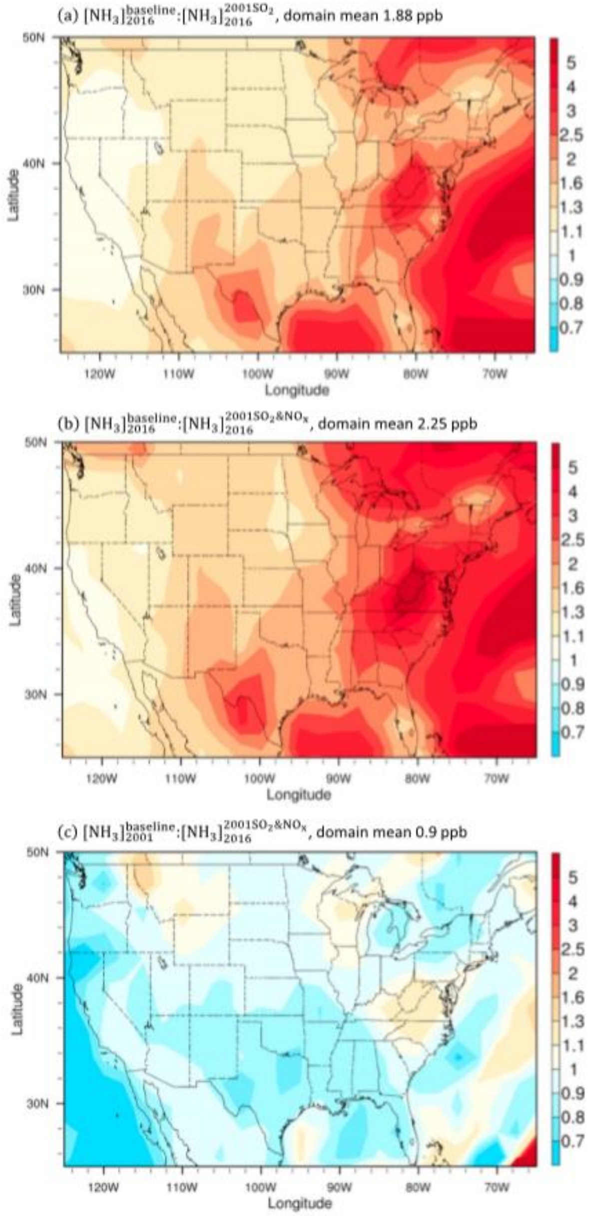


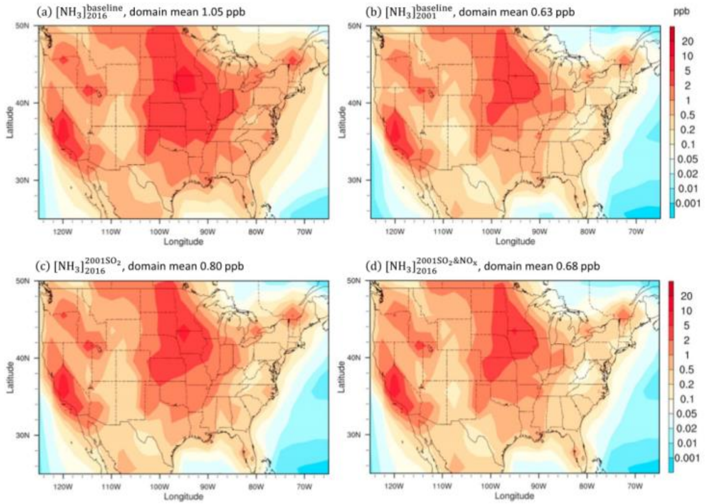




Long-Term Trend of Gaseous Ammonia Over the United States: Modeling and Comparison With Observations

- Sensitivity of [NH3] to SO2 and NOx Emissions
  - The effect of SO2 and NOx emissions on simulated annual mean [NH3] in the model surface layer
    - SO2 contributes to about 2/3 and NOx to 1/3 of the changes in [NH3]
  - ratios of $[NH_3]_{2016}^{baseline}$ to $[NH_3]_{2016}^{2001SO_2}$, $[NH_3]_{2016}^{baseline}$ to $[NH_3]_{2016}^{2001SO_2\&NO_x}$, $[NH_3]_{2001}^{baseline}$ to $[NH_3]_{2016}^{2001SO_2\&NO_x}$.
    - if emissions of (a) SO2 only and (b) both SO2 and NOx remained unchanged over the 16-year period, current [NH3] over the United States would be significantly lower, by a factor of ~1.88 and ~2.25

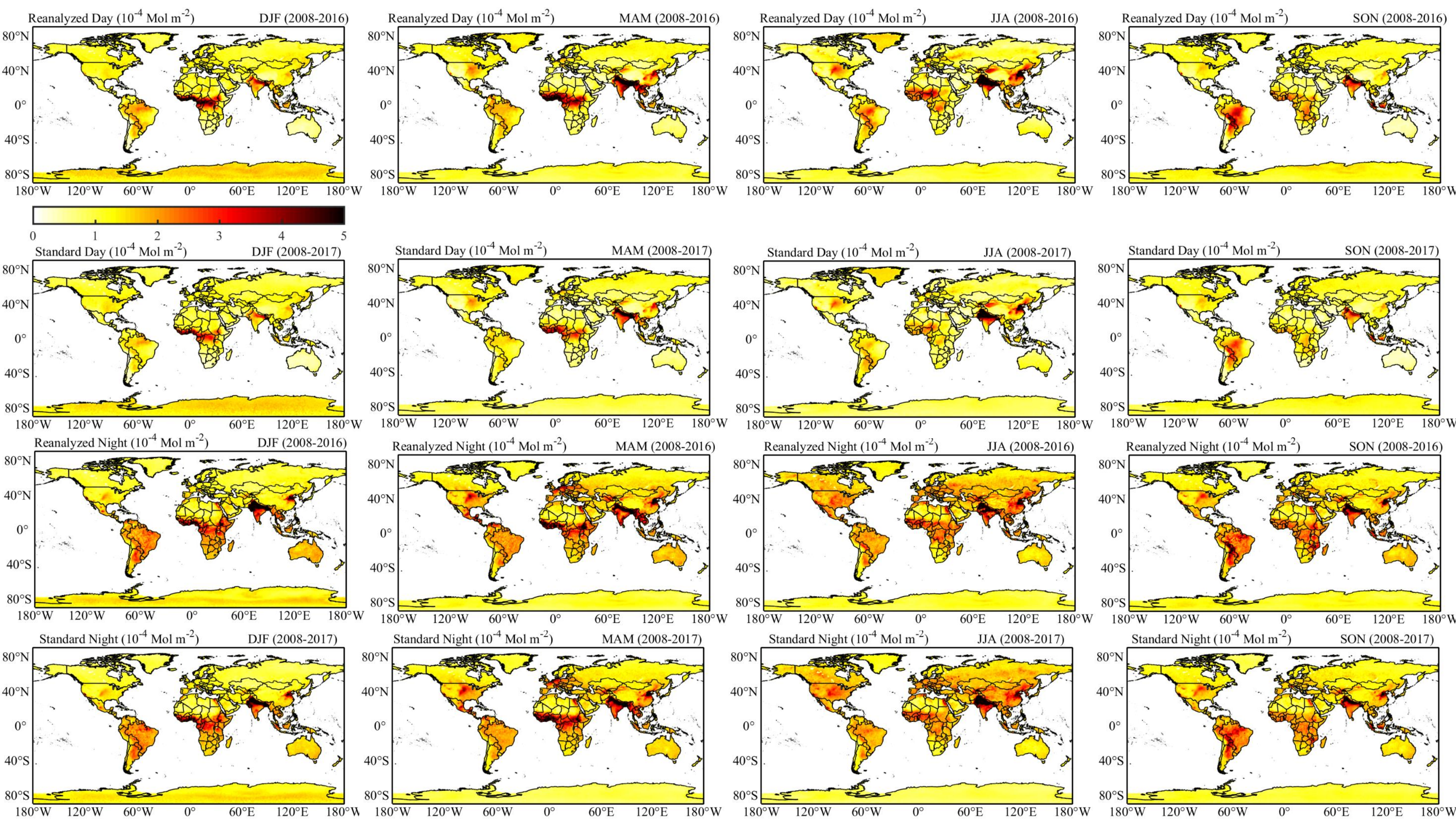




(Yu et al, 2018)

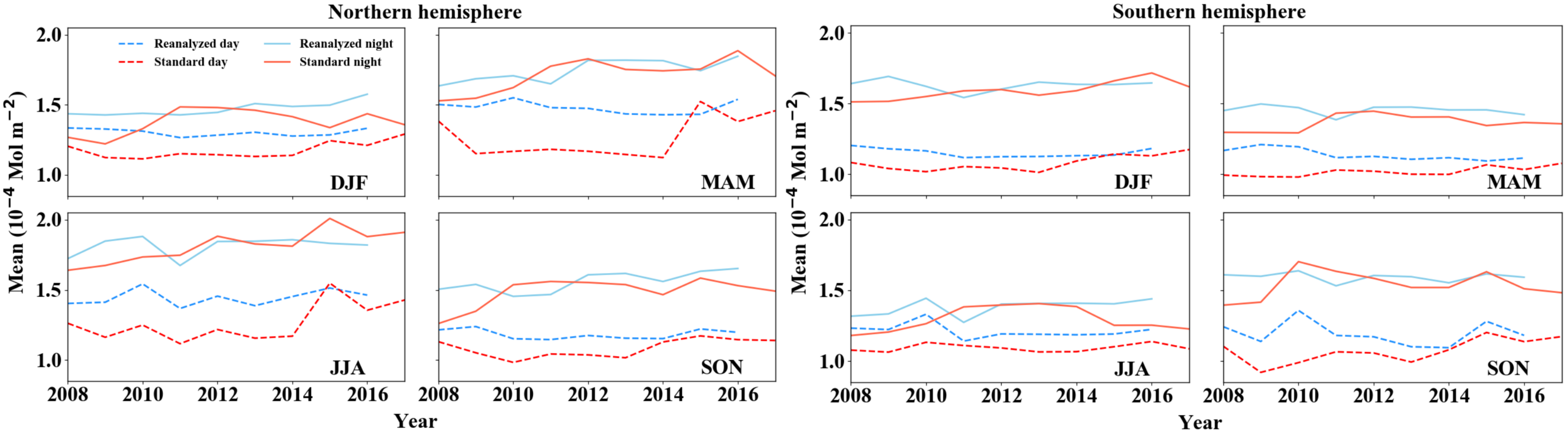
Spatial distribution of ammonia observations mean

- Reanalyzed 2008-2016: row 1, 3
- Standard 2008-2017: row 2, 4
- DJF: col 1
- MAM: col 2
- JJA: col 3
- SON: col 4
- Day: row 1, 2
- Night: row 3, 4

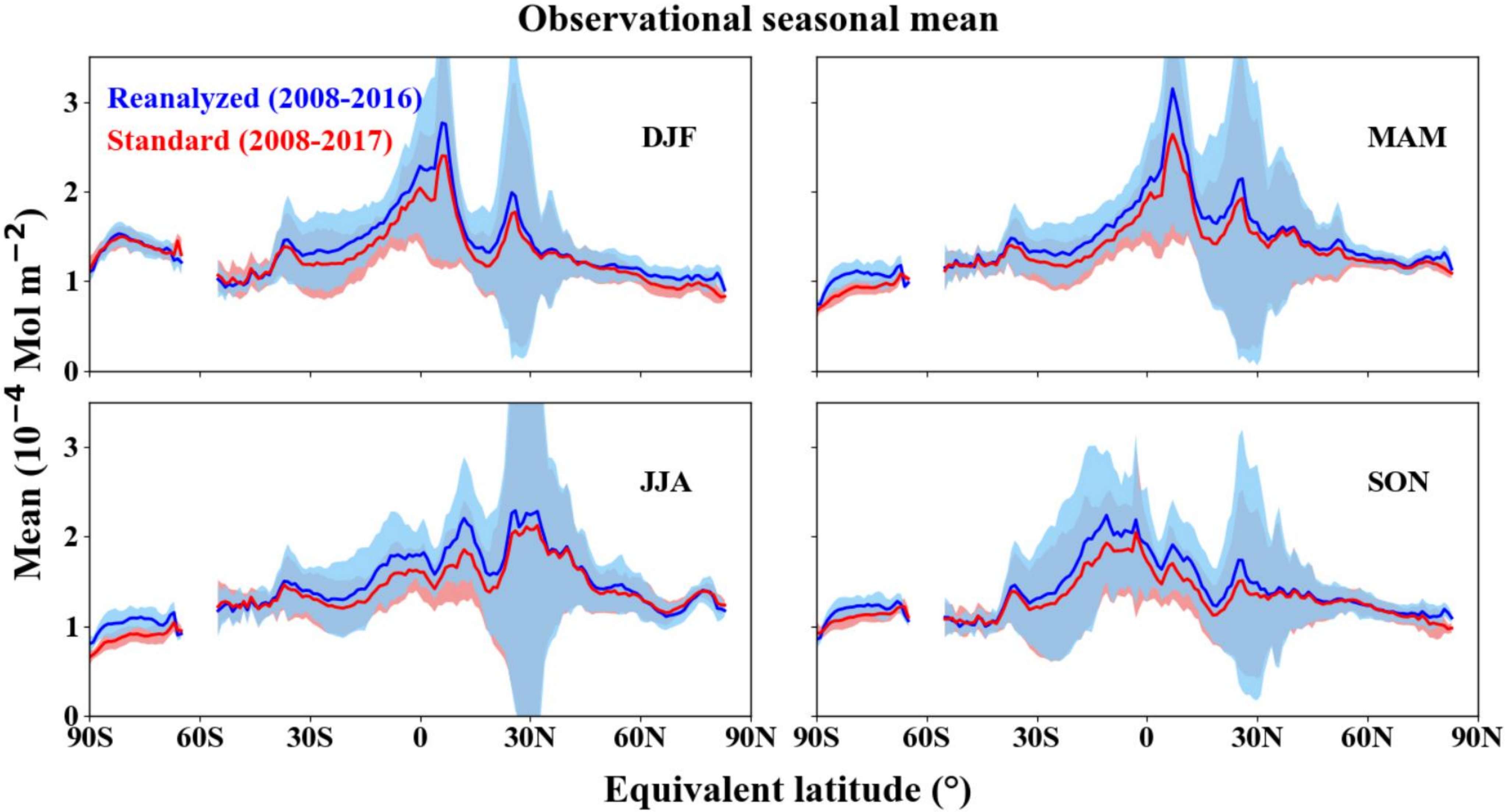


Reanalyzed Day (10^{-4} Mol m^{-2}) DJF (2008-2016)
Reanalyzed Day (10^{-4} Mol m^{-2}) MAM (2008-2016)
Reanalyzed Day (10^{-4} Mol m^{-2}) JJA (2008-2016)
Reanalyzed Day (10^{-4} Mol m^{-2}) SON (2008-2016)
0 1 2 3 4 5
Standard Day (10^{-4} Mol m^{-2}) DJF (2008-2017)
Standard Day (10^{-4} Mol m^{-2}) MAM (2008-2017)
Standard Day (10^{-4} Mol m^{-2}) JJA (2008-2017)
Standard Day (10^{-4} Mol m^{-2}) SON (2008-2017)
Reanalyzed Night (10^{-4} Mol m^{-2}) DJF (2008-2016)
Reanalyzed Night (10^{-4} Mol m^{-2}) MAM (2008-2016)
Reanalyzed Night (10^{-4} Mol m^{-2}) JJA (2008-2016)
Reanalyzed Night (10^{-4} Mol m^{-2}) SON (2008-2016)
Standard Night (10^{-4} Mol m^{-2}) DJF (2008-2017)
Standard Night (10^{-4} Mol m^{-2}) MAM (2008-2017)
Standard Night (10^{-4} Mol m^{-2}) JJA (2008-2017)
Standard Night (10^{-4} Mol m^{-2}) SON (2008-2017)
80°N 40°N 0° 40°S 80°S
180°W 120°W 60°W 0° 60°E 120°E 180°W

Seasonal change for NH and SH (day and night)

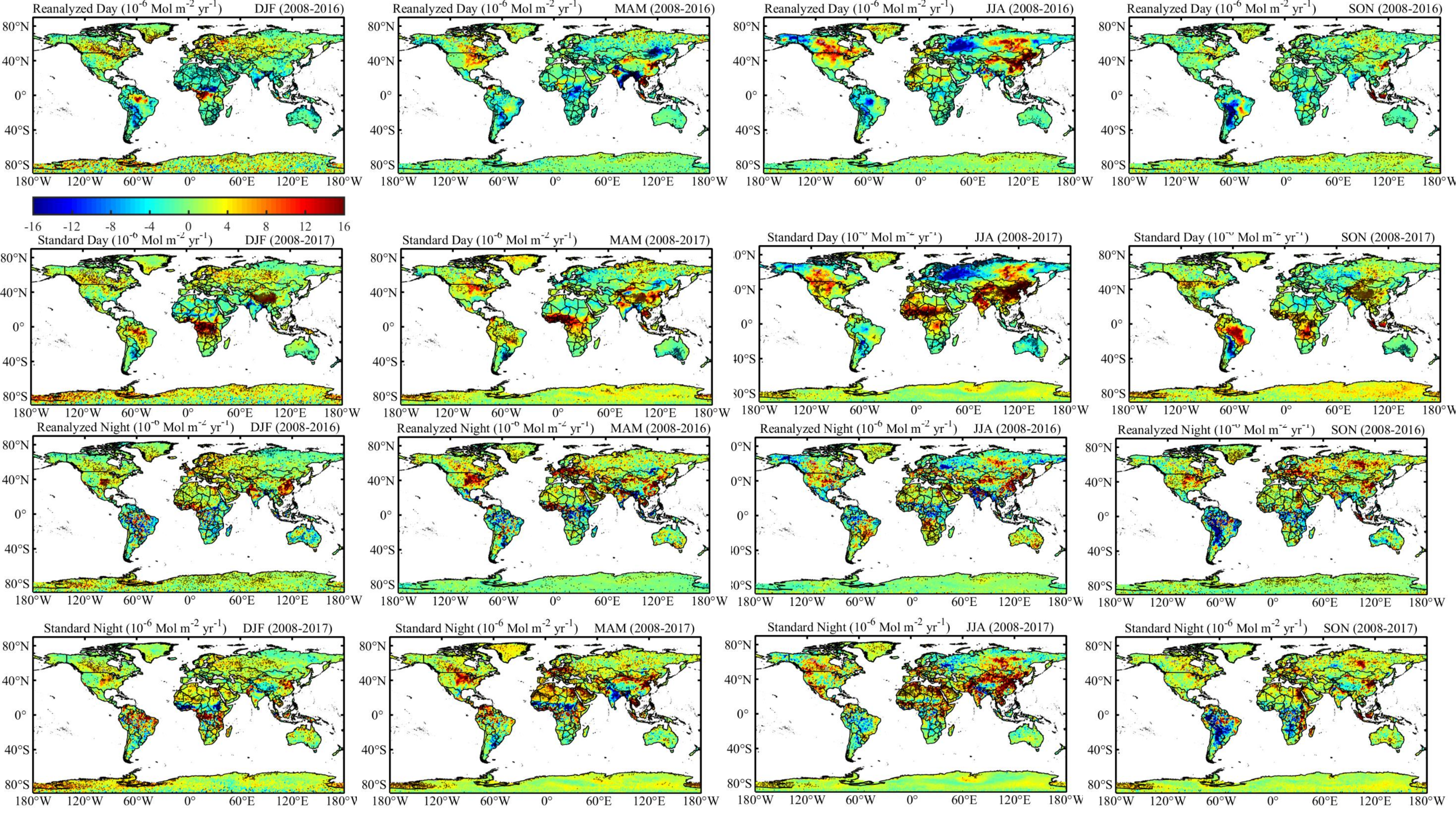


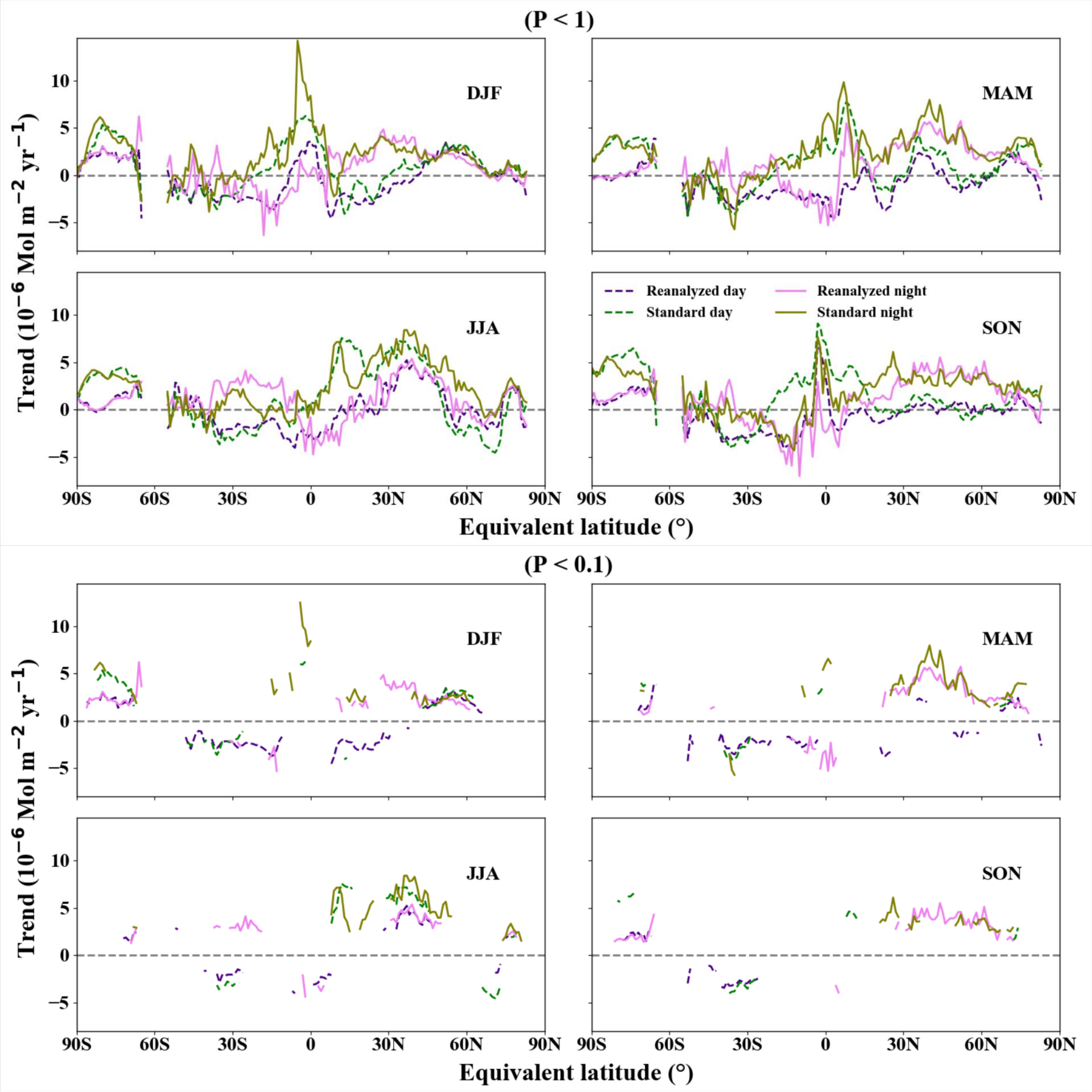
Seasonal mean of Land for equivalent latitude (within 1 sigma standard deviations)



Spatial distribution of ammonia observations trend

- Reanalyzed 2008-2016: row 1, 3
- Standard 2008-2017: row 2, 4
- DJF: col 1
- MAM: col 2
- JJA: col 3
- SON: col 4
- Day: row 1, 2
- Night: row 3, 4

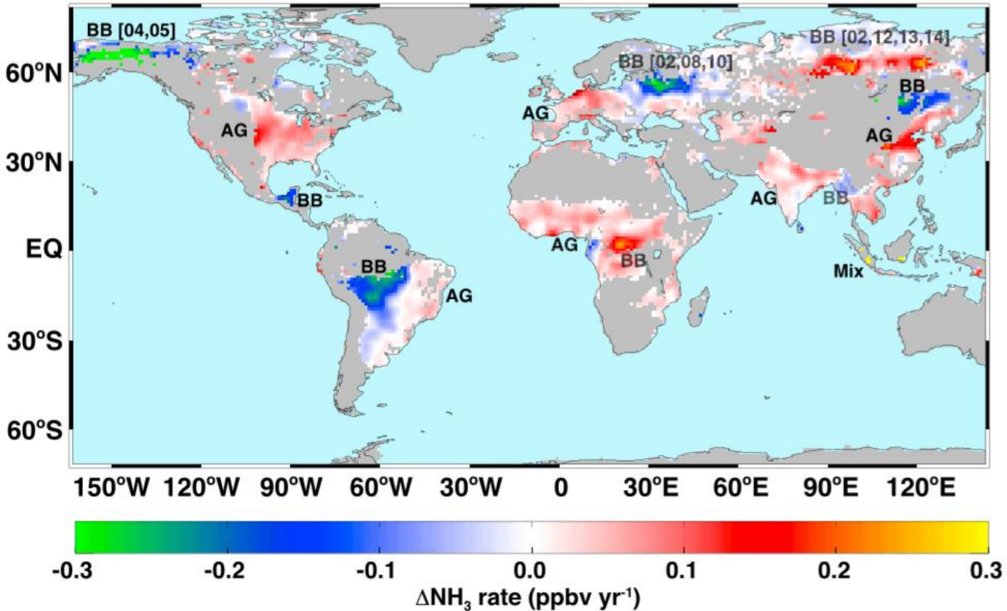

Reanalyzed Day (10-6 Mol m-2 yr-1) DJF (2008-2016)
Reanalyzed Day (10-6 Mol m-2 yr-1) MAM (2008-2016)
Reanalyzed Day (10-6 Mol m-2 yr-1) JJA (2008-2016)
Reanalyzed Day (10-6 Mol m-2 yr-1) SON (2008-2016)
-16 -12 -8 -4 0 4 8 12 16
Standard Day (10-6 Mol m-2 yr-1) DJF (2008-2017)
Standard Day (10-6 Mol m-2 yr-1) MAM (2008-2017)
Standard Day (10-6 Mol m-2 yr-1) JJA (2008-2017)
Standard Day (10-6 Mol m-2 yr-1) SON (2008-2017)
Reanalyzed Night (10-6 Mol m-2 yr-1) DJF (2008-2016)
Reanalyzed Night (10-6 Mol m-2 yr-1) MAM (2008-2016)
Reanalyzed Night (10-6 Mol m-2 yr-1) JJA (2008-2016)
Reanalyzed Night (10-6 Mol m-2 yr-1) SON (2008-2016)
Standard Night (10-6 Mol m-2 yr-1) DJF (2008-2017)
Standard Night (10-6 Mol m-2 yr-1) MAM (2008-2017)
Standard Night (10-6 Mol m-2 yr-1) JJA (2008-2017)
Standard Night (10-6 Mol m-2 yr-1) SON (2008-2017)
80°N 40°N 0° 40°S 80°S
180°W 120°W 60°W 0° 60°E 120°E 180°W



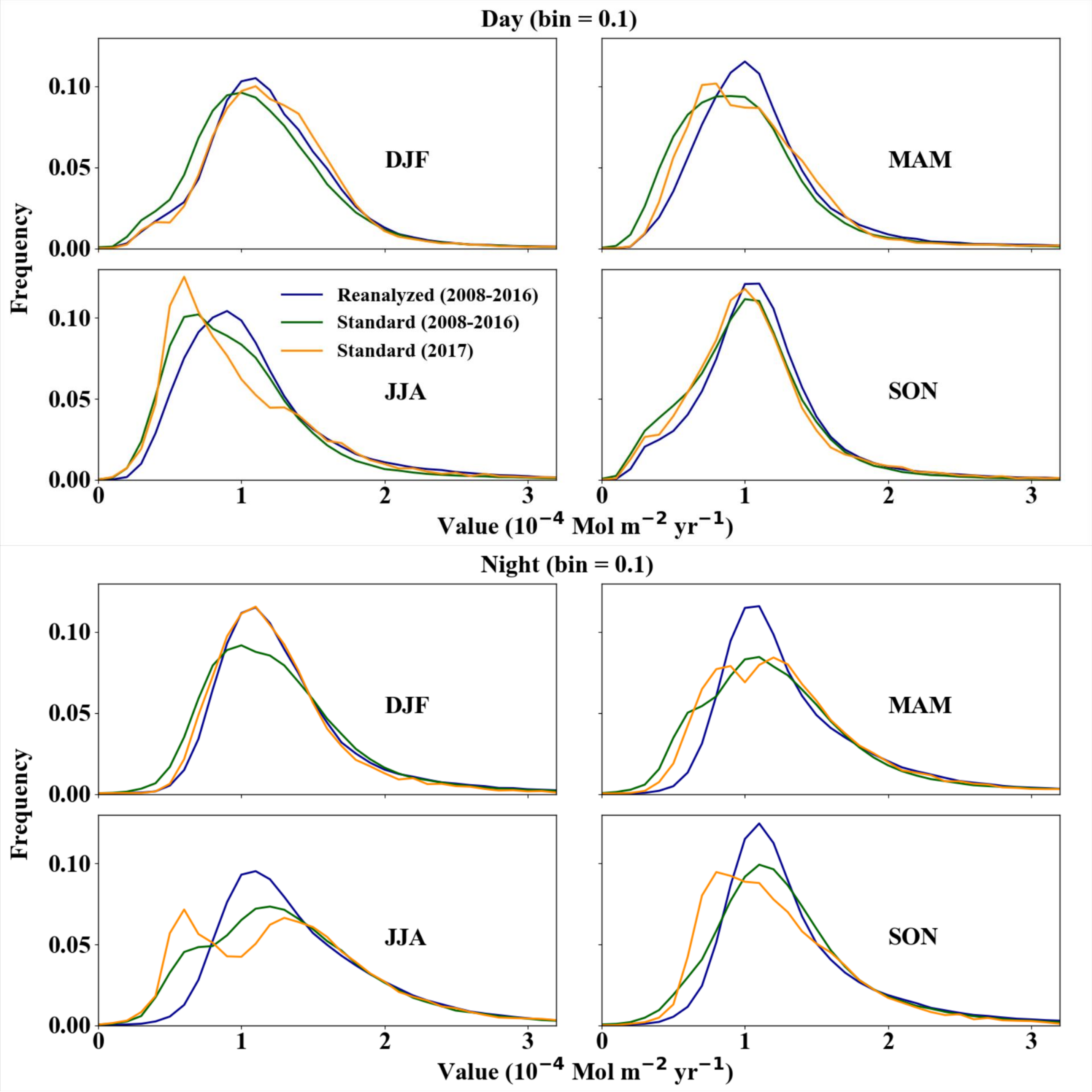
Seasonal trend in the equivalent latitude over 2008-2016 (day and night)

Increased atmospheric ammonia over the world's major agricultural areas detected from space

- provides evidence of substantial increases in atmospheric ammonia (NH3) concentrations (14year) over several of the worlds major agricultural regions
- The rate of change of NH3 volume mixing ratio (VMR) in parts-per-billion by volume (ppbv) per year computed
  - BB: biomass burning
  - AG: agricultural

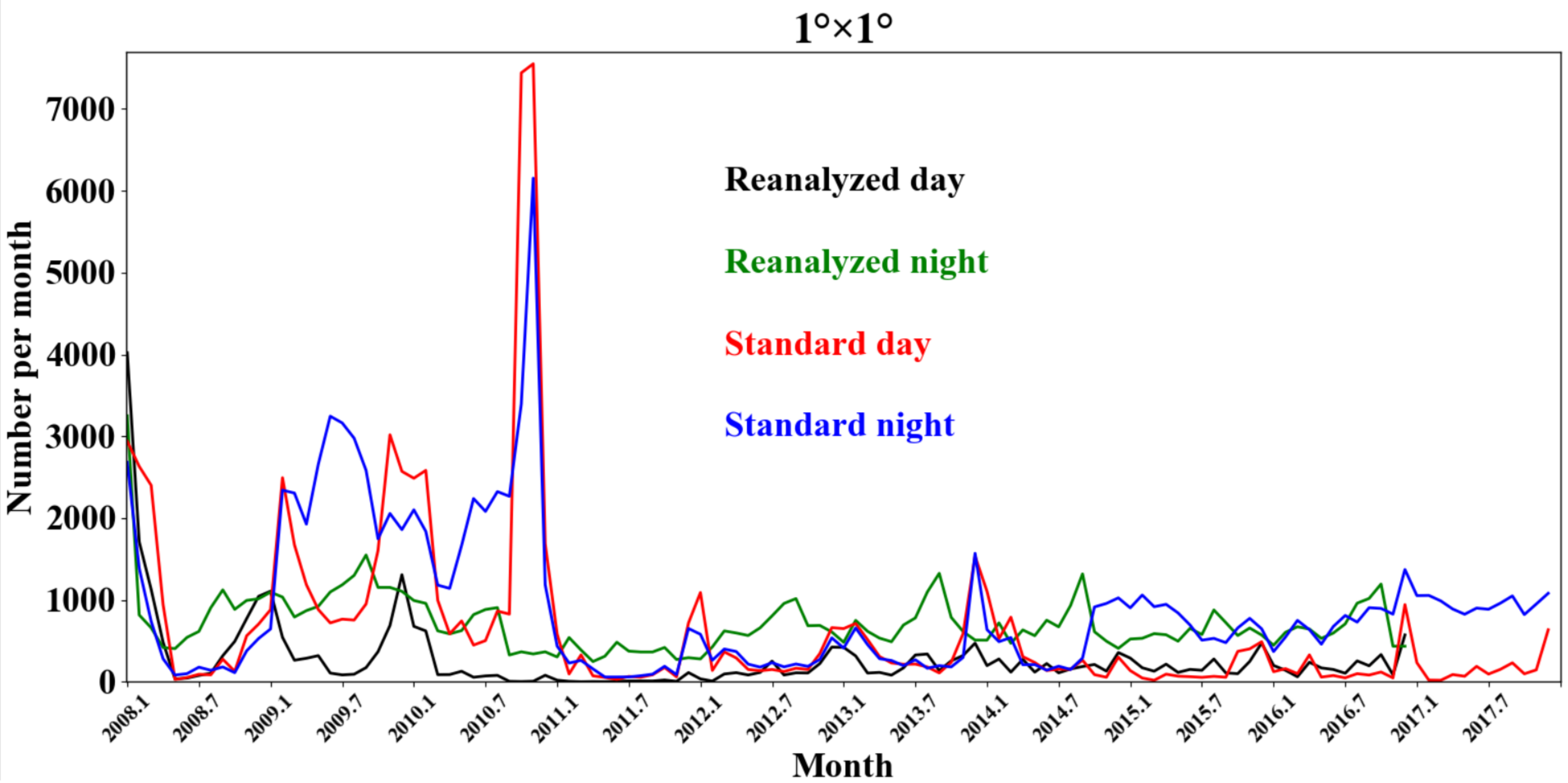


(Warner et al, 2016)



PDF of the 2008-2016 and 2017 (day and night)

Missing value of datasets over 2008-2017 (per month)



GEO-Chem

GEOS-Chem simulation

- 4°x5° "standard" simulation
  - Memory: 8+ GB RAM
  - Disk: ~30 GB/yr
  - Version: 12.9.3
- Editing the CopyRunDirs.input file
  - UnitTest.input: all possible run directories can add
    - GEOS-Chem benchmark: benchmark
    - Transport Tracers: TransportTracers
    - Mercury, Tagged Mercury: Hg
    - POPs: tagHg
    - Methane: POPs
    - Tagged O3: CH4
    - Tagged CO: tagO3
    - Carbon Dioxide: tagCO
    - Carbon Dioxide: CO2
    - Offline Aerosols: aerosol
    - Standard: standard
    - Tropchem: tropchem
    - Complex SOA: complexSOA/complexSOA_SVPOA
    - Acid uptake on dust: aciduptake
    - Marine POA: marinePOA
    - APM aerosol microphysics: APM
    - TOMAS aerosol microphysics: TOMAS15/TOMAS40

GEOS-Chem simulation

- Editing the CopyRunDirs.input file
  - Section 1: INPUTS
    - Version: An ID tag
    - DESCRIPTION: the purpose of this specific file
    - DATA_ROOT: root-level data directory
    - HEMCO_ROOT: the top-level path for the HEMCO data directory tree
    - VERBOSE: the level of debug output (0-3)
    - WARNINGS: the level of warning messages (0-3)
    - UNIT_TEST_ROOT: the path to the GEOS-Chem Unit Tester
    - RUN_ROOT: the top-level unit test run directories
    - RUN_DIR: the run directory subdirectory
    - PERL_DIR: the directory where the unit test Perl scripts are found
    - COPY_PATH: the directory on your disk server where copies of the GEOS-Chem run directories will be created
    - COPY_CMD: the command used to copy run directories from the GEOS-Chem Unit Tester to COPY_PATH
      - cp –rfL: create a new copy of the directory
      - cp –L: create "hard" copies of files that are symbolic links (differ)

GEOS-Chem simulation

- Editing the CopyRunDirs.input file
  - Section 2: RUNS
    - met fields uesed
    - GEOS-Chem horizontal grid
    - GEOS-Chem simulation item
    - Starting time
    - Ending time

```
## ======= Tropchem ================================================
# geosfp   4x5        -      tropchem        2016070100   2016080100     -
  merra2   4x5        -      tropchem        2010010100   2011010100     -
```

- Generating a GEOS-Chem Run Directory
  - Once edited: type ./gcCopyRunDirs
  - create a new GEOS-Chem run directory
- configuration files
  - User inputs
    - input.geos
      - Simulation: Start & end time
      - Grid: definitions
      - Timestep: from minutes to seconds
      - Advected Species: The type of GEOS-Chem simulation that perform
      - Transport: TPCORE
      - Convection: cloud convection, PBL mixing,
      - Emissions:
      - Aerosols
      - Deposition
      - Chemistry
      - Planeflight diagnostic
      - ObsPack diagnostic
      - ND51 and ND51b diagnostics: satellite timeseries diagnostics
      - Passive Species Menu

GEOS-Chem simulation

- configuration files
  - User inputs
    - HEMCO_Config.rc: emission inventories, Enabling and disabling emissions
      - GEIA_NH3
      - SEABIRD_NH3
    - HEMCO_Diagn.rc: diagnostic archival options for emissions and related quantities
    - HISTORY.rc: which GEOS-Chem diagnostics will be archived to netCDF output

GEOS-Chem simulation

- Compiling
  - Cmake: a platform-independent build system
    - Obtaining Cmake: /pdiskdata/zhangyuzhonggroup/zhangyuzhong/Software/bin
    - Compiling GEOS-Chem "Classic" with Cmake
      - Run directory contents
        - CodeDir: a symbolic link to the code directory
        - Makefile: the run-directory Makefile
        - OutputDir: where diagnostic files will be placed
        - input.geos/*.rc: configuration files
        - download_data.py: data download script for the GEOS-Chem dry-run simulation
        - validate.pl: only used for GEOS-Chem unit tests and difference tests (ignore)
      - Create a build subfolder in your run directory
        - Build directory used to compile GEOS-Chem: mkdir Subbuild
        - switch to the Subbuild folder: configure and build GEOS-Chem
      - Configure the build (gcbuild folder)
        - Configuring with default options: cmake ../CodeDir (failed, version `GLIBCXX_3.4.14' not found)
      - Compiling the code

GEOS-Chem simulation

- Compiling
  - GNU Make (retired after 13.0)
    - Compiling GEOS-Chem "Classic"

```
OPTIONAL-FLAGS may be one of the following:
-----------------------------------------------------------
DEBUG=y              Compiles GEOS-Chem with various debugging options
BOUNDS=y             Compiles GEOS-Chem with out-of-bounds error checks
FPE=y                Compiles GEOS-Chem with floating-point math error checks
TRACEBACK=y          Compiles GEOS-Chem with traceback error printout (this is the default)
```

      - Determining available compilation options: make help
      - Clean up files in the run directory: make cleanup_output
      - Build the GEOS-Chem executable: make -j4 build [option]
      - Log files created by the compilation
        - compile.log: Contains echo-back of the GEOS-Chem compilation output
        - lastbuild: Contains a summary of all of the options that were used to build the GEOS-Chem executable

- Running
  - qlogin (test)
  - qsub [options] job.sh:
  - qstat
  - qstat -g c
  - qdel