

# Ammonia observation and modeling simulation 3

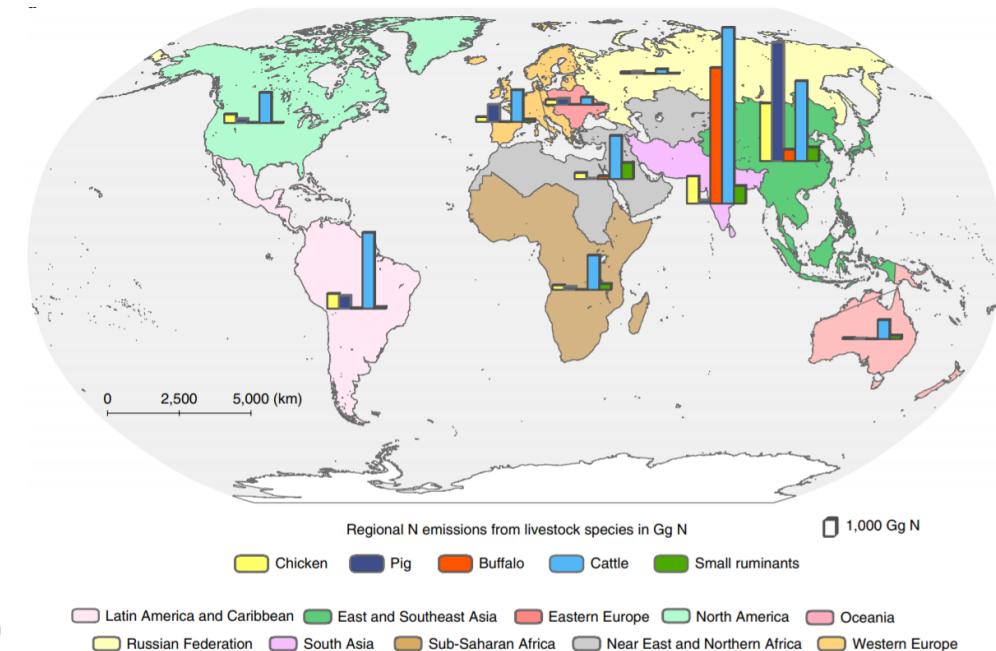
IASI data and GEOS-Chem model

2020.10

- Accomplished:
  - 1. literature: global nitrogen emissions from livestock chain
  - 2. literature: global nitrous oxide budget
  - 3. literature: nitrous oxide emission of livestock enclosures in Sub-Saharan Africa
  - 3. literature: Industrial and agricultural ammonia point sources
  - 4. literature: improved nitrogen use efficiency scenarios in China
  - 5. fix the floating invalid bug of GEOS-Chem
  - 6. 2010.1-2010.2 output from GEOS-Chem
  - 7. Simulating GEOS-Chem Tropchem manual
- Ammonia Data:
  - IASI (2008-2016),  $1^\circ \times 1^\circ$ , monthly, land area
    - Reanalyzed IASI/Metop-A (2008-2016) L3
- Ongoing:
  - 1. running the GEOS-Chem Tropchem over 2010
  - 2. calculating the column concentration from GEOS-Chem output (47 levels integration)

# Nitrogen emissions along global livestock supply chains

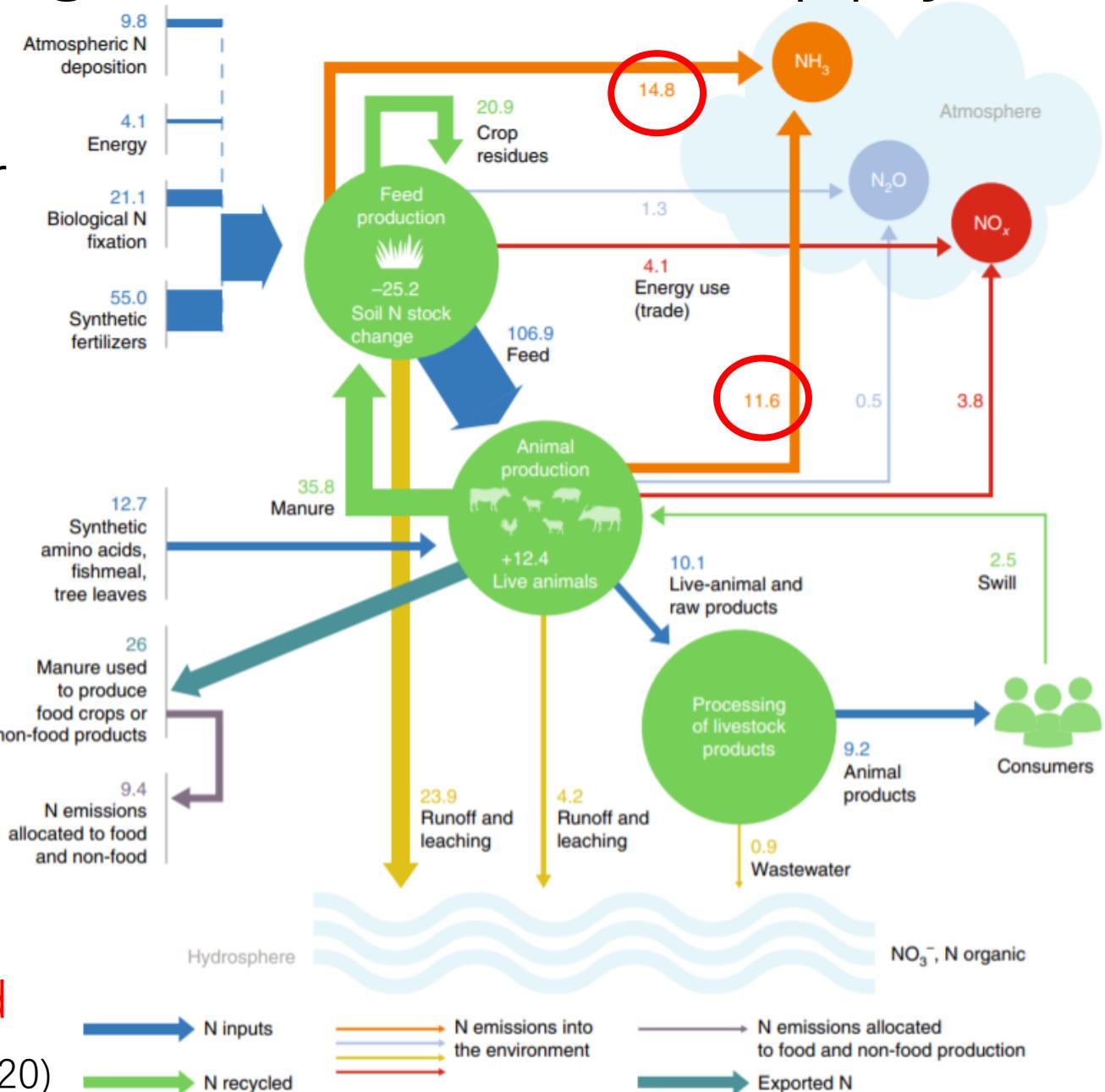
- highlight the diversity of livestock supply chains and international trade.
- quantify N-use indicators of life-cycle nitrogen use efficiency and life-cycle net nitrogen balance
- identify hotspots of N emissions and ultimately suggesting targeted interventions to reduce emissions



# Nitrogen emissions along global livestock supply chains

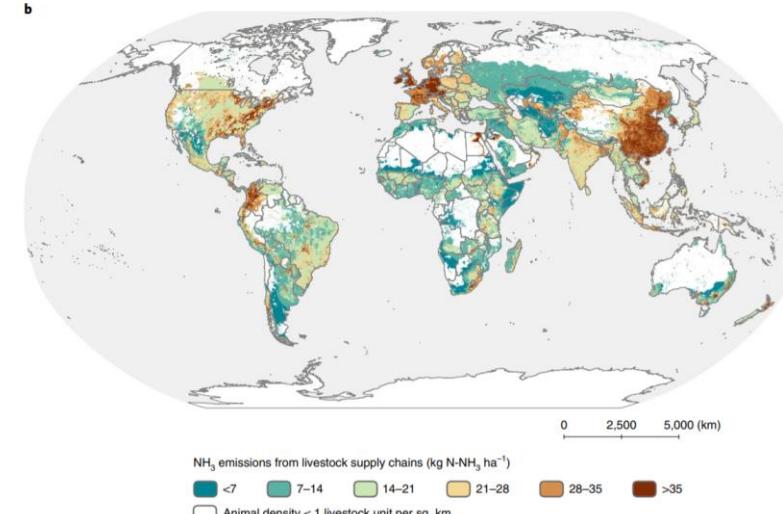
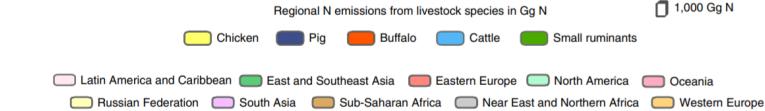
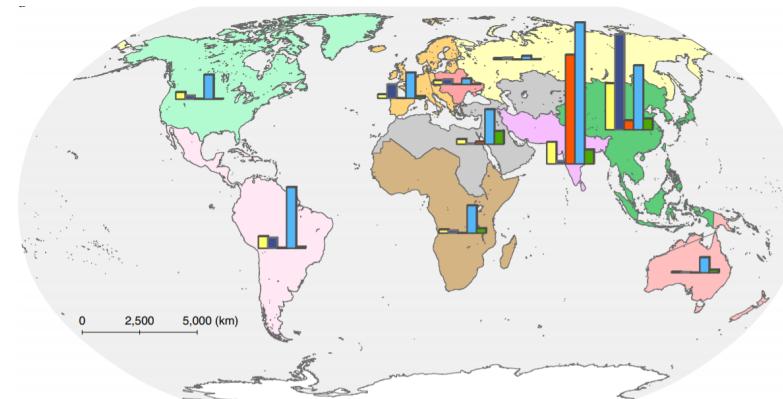
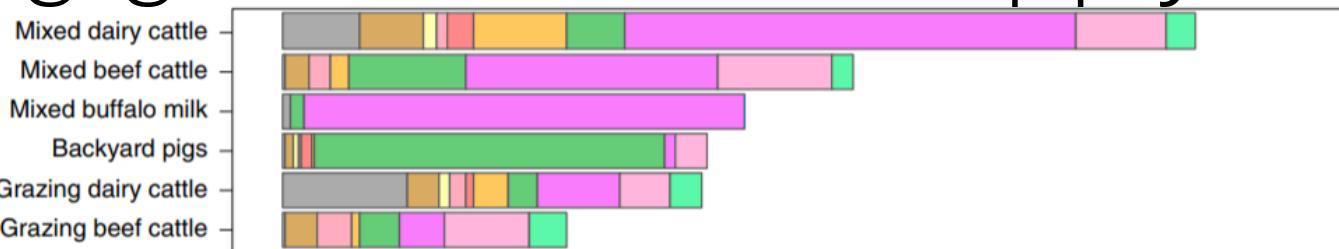
- N emissions from the livestock sector
  - Global N flows and sources of N compound emissions allocated to the livestock sector: **livestock supply chains contributed 25.4 Tg N to Atmosphere**
    - 14.8 from feed production
    - 11.6 from animal production
- N emissions per supply chain
  - Distribution of N emissions by livestock species for 10 regions: South Asia, East and Southeast Asia and Latin America and the Caribbean given the high numbers of livestock held in **mixed and grazing ruminant systems and backyard monogastric systems**

(Uwizeye et al., 2020)



# Nitrogen emissions along global livestock supply chains

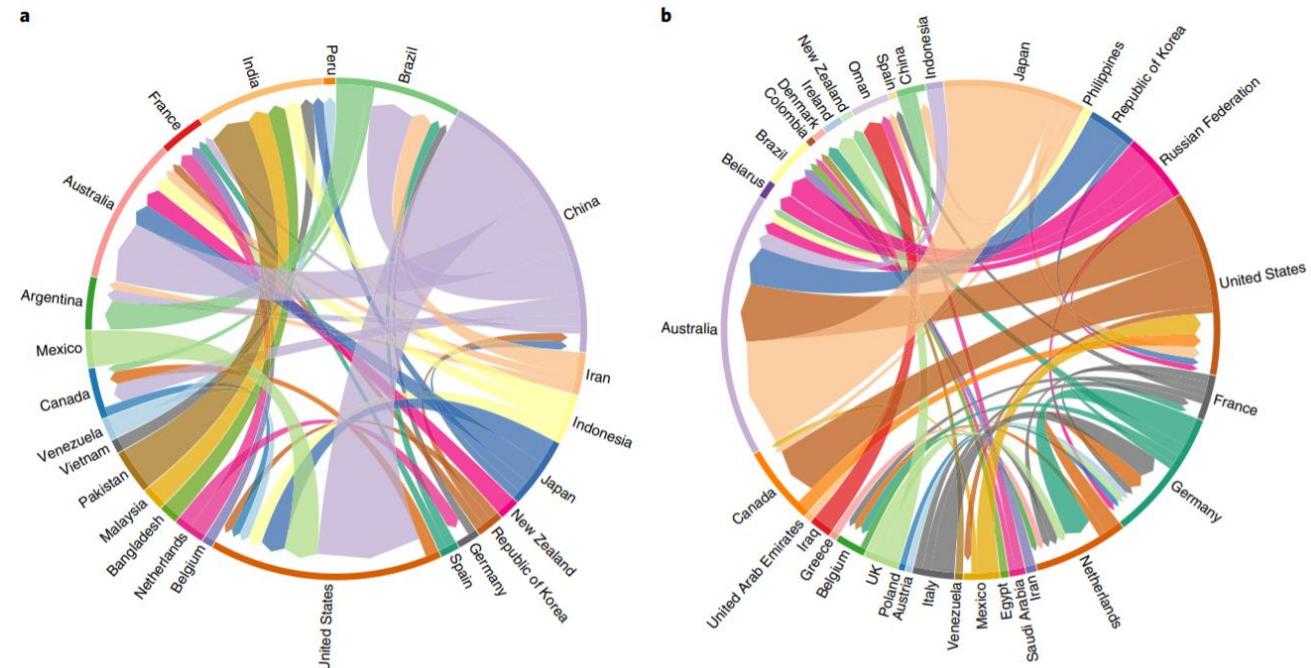
- N emissions per supply chain
  - mixed cattle and buffalo supply chains alone are responsible for **44%** of the total N emissions
- Regional hotspots of N emissions
  - Most N emissions take place in the regions of **South Asia, East and Southeast Asia and Latin America and the Caribbean**
  - NH<sub>3</sub> emissions are concentrated in **East and Southeast Asia, East Australia and New Zealand, Western Europe, Colombia, east coast of the United States and the Nile Delta**



# Nitrogen emissions along global livestock supply chains

- N emissions from domestic consumption

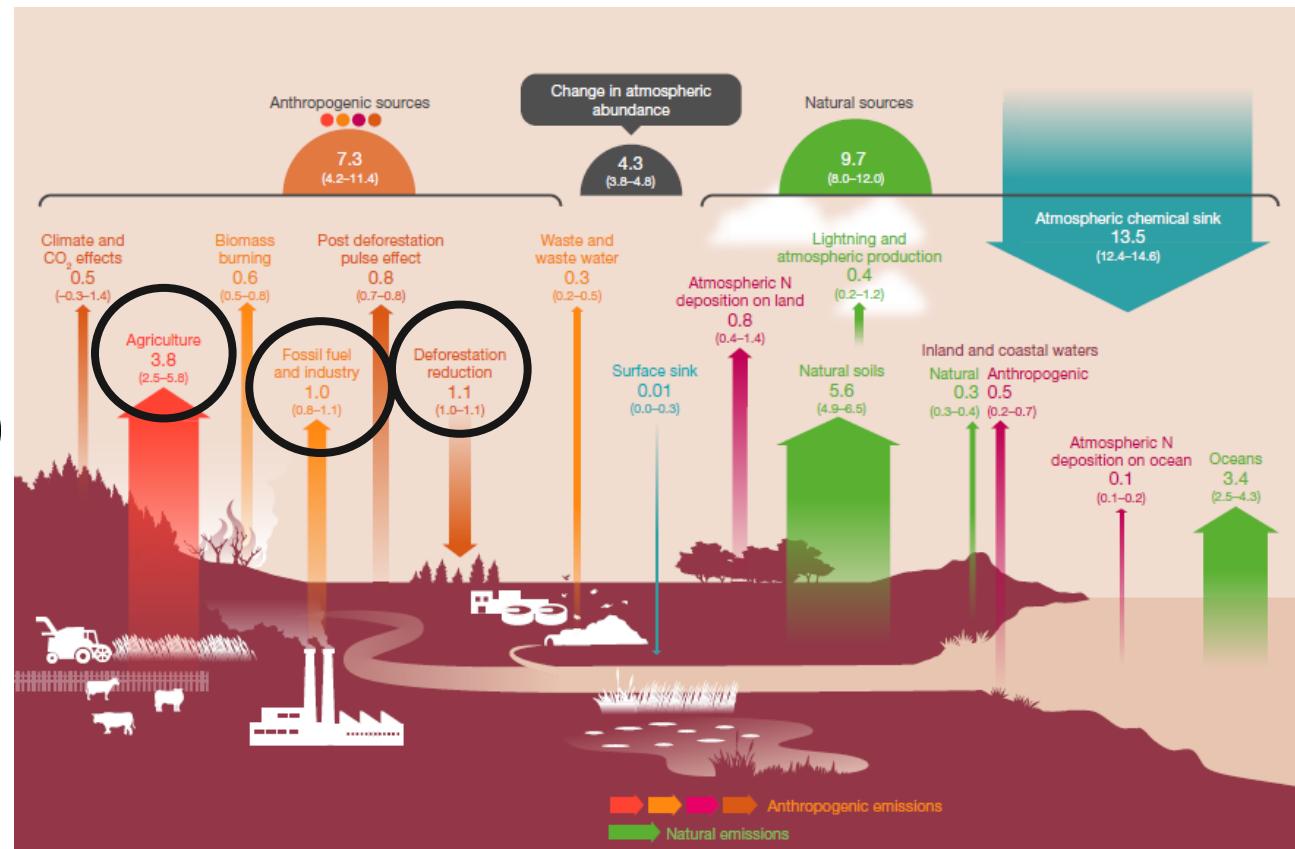
- Feed commodities relate mostly to the fertilization of feed, 59% is associated with the trade of cereals, 39% with soybean and soybean cake and 2% with the trade in palm products and cassava
- Livestock commodities stem from the production of beef (41%), milk (31%), pork (15%), chicken meat (8%), sheep meat (3%) and eggs (1%).



(Uwizeye et al., 2020)

# A comprehensive quantification of global nitrous oxide sources and sinks

- constructed a total of 43 flux estimates:
  - 30 using bottom-up approaches,
  - 5 using top-down approaches,
  - 8 other estimates using **observation and modelling** approaches
- The global N<sub>2</sub>O budget (2007–2016)
  - **Anthropogenic sources contributed 43%** to the total N<sub>2</sub>O emission of which direct and indirect emissions from nitrogen additions **in agriculture** and other sectors contributed around **52%** and around **18%**, respectively.



(Tian et al., 2020)

# A comprehensive quantification of global nitrous oxide sources and sinks

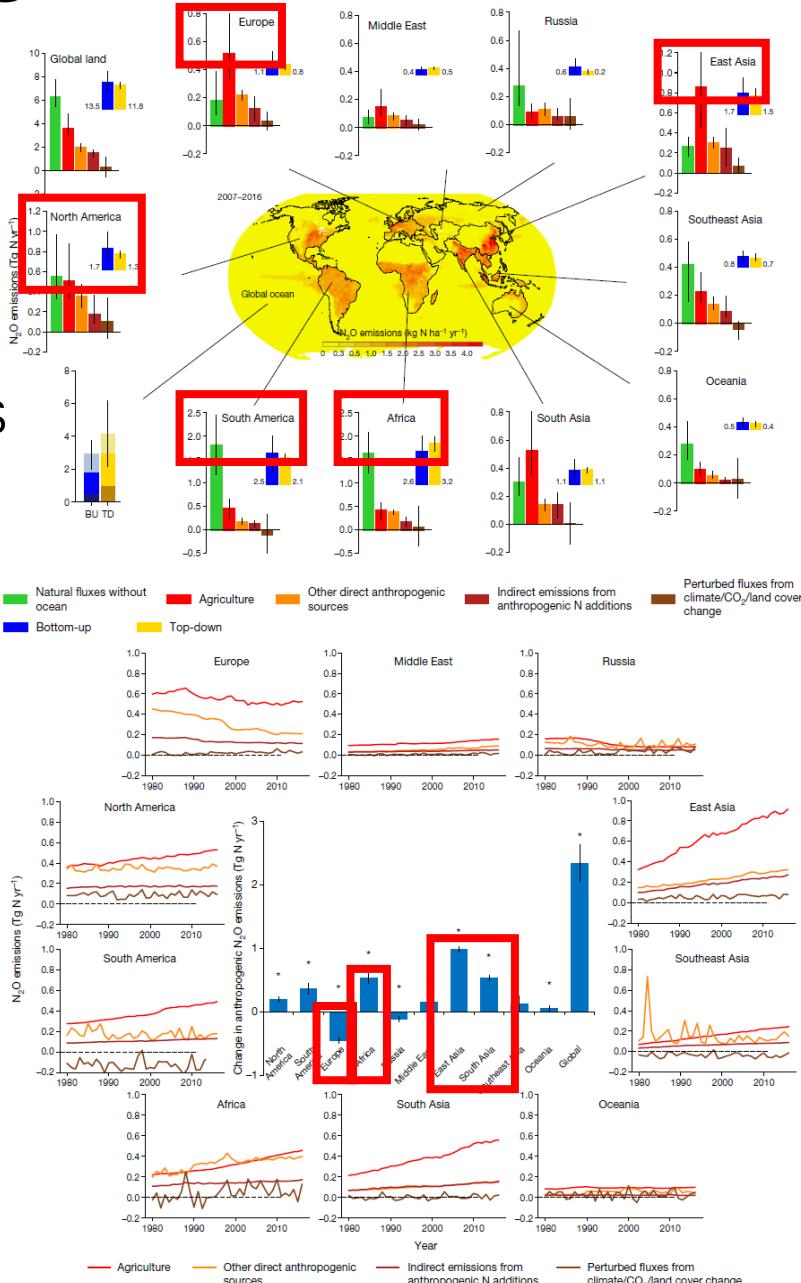
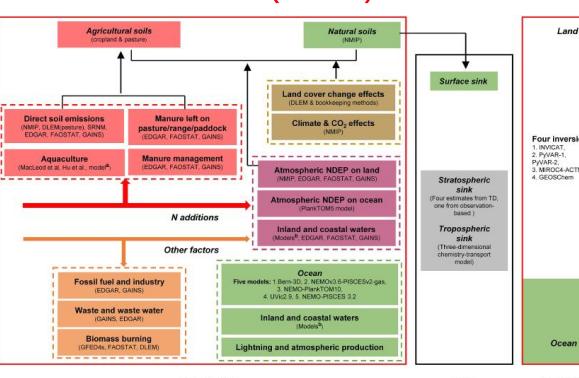
- Four decades of the global N<sub>2</sub>O budget
    - a substantial increase in global N<sub>2</sub>O emissions that is primarily driven by anthropogenic sources, as natural sources remained relatively steady throughout the study period.
    - recent climate change—particularly warming could have boosted soil nitrification and denitrification processes, contributing to the growing trend in N<sub>2</sub>O emissions together with increasing nitrogen additions to agricultural soils

|   | 1980s  |            |             | 1990s      |            |             | 2000s      |            |             | 2007–2016   |            |             |             |
|---|--|------------|-------------|------------|------------|-------------|------------|------------|-------------|-------------|------------|-------------|-------------|
| Anthropogenic sources   | Mean   | Min.       | Max.        | Mean       | Min.       | Max.        | Mean       | Min.       | Max.        | Mean        | Min.       | Max.        |             |
| Direct emissions from nitrogen additions in the agricultural sector (Agriculture) | Direct soil emissions                          | 1.5        | 0.9         | 2.6        | 1.7        | 1.1         | 3.1        | 2.0        | 1.3         | 3.4         | 2.3        | 1.4         | 3.8         |
|   | Manure left on pasture                         | 0.9        | 0.7         | 1.0        | 1.0        | 0.7         | 1.1        | 1.1        | 0.8         | 1.2         | 1.2        | 0.9         | 1.3         |
|   | Manure management                              | 0.3        | 0.2         | 0.4        | 0.3        | 0.2         | 0.4        | 0.3        | 0.2         | 0.5         | 0.3        | 0.2         | 0.5         |
|   | Aquaculture                                    | 0.01       | 0.00        | 0.03       | 0.03       | 0.01        | 0.1        | 0.1        | 0.02        | 0.2         | 0.1        | 0.02        | 0.2         |
|   | <b>Subtotal</b>                                | <b>2.6</b> | <b>1.8</b>  | <b>4.1</b> | <b>3.0</b> | <b>2.1</b>  | <b>4.8</b> | <b>3.4</b> | <b>2.3</b>  | <b>5.2</b>  | <b>3.8</b> | <b>2.5</b>  | <b>5.8</b>  |
| Other direct anthropogenic sources  | Fossil fuels and industry                      | 0.9        | 0.8         | 1.1        | 0.9        | 0.9         | 1.0        | 0.9        | 0.8         | 1.0         | 1.0        | 0.8         | 1.1         |
|   | Waste and waste water                          | 0.2        | 0.1         | 0.3        | 0.3        | 0.2         | 0.4        | 0.3        | 0.2         | 0.4         | 0.3        | 0.2         | 0.5         |
|   | Biomass burning                                | 0.7        | 0.7         | 0.7        | 0.7        | 0.6         | 0.8        | 0.6        | 0.6         | 0.6         | 0.6        | 0.5         | 0.8         |
|   | <b>Subtotal</b>                                | <b>1.8</b> | <b>1.6</b>  | <b>2.1</b> | <b>1.9</b> | <b>1.7</b>  | <b>2.1</b> | <b>1.8</b> | <b>1.6</b>  | <b>2.1</b>  | <b>1.9</b> | <b>1.6</b>  | <b>2.3</b>  |
| Indirect emissions from anthropogenic nitrogen additions                          | Inland waters, estuaries, coastal zones        | 0.4        | 0.2         | 0.5        | 0.4        | 0.2         | 0.5        | 0.4        | 0.2         | 0.6         | 0.5        | 0.2         | 0.7         |
|   | Atmospheric nitrogen deposition on land        | 0.6        | 0.3         | 1.2        | 0.7        | 0.4         | 1.4        | 0.7        | 0.4         | 1.3         | 0.8        | 0.4         | 1.4         |
|   | Atmospheric nitrogen deposition on ocean       | 0.1        | 0.1         | 0.2        | 0.1        | 0.1         | 0.2        | 0.1        | 0.1         | 0.2         | 0.1        | 0.1         | 0.2         |
|   | <b>Subtotal</b>                                | <b>1.1</b> | <b>0.6</b>  | <b>1.9</b> | <b>1.2</b> | <b>0.7</b>  | <b>2.1</b> | <b>1.2</b> | <b>0.6</b>  | <b>2.1</b>  | <b>1.3</b> | <b>0.7</b>  | <b>2.2</b>  |
|   |  |            |             |            |            |             |            |            |             |             |            |             |             |
| Perturbed fluxes from climate/CO <sub>2</sub> /land cover change                  | CO <sub>2</sub> effect                         | -0.2       | -0.3        | 0.0        | -0.2       | -0.4        | 0.0        | -0.3       | -0.5        | 0.1         | -0.3       | -0.6        | 0.1         |
|   | Climate effect                                 | 0.4        | 0.0         | 0.8        | 0.5        | 0.1         | 0.9        | 0.7        | 0.3         | 1.2         | 0.8        | 0.3         | 1.3         |
|   | Post-deforestation pulse effect                | 0.7        | 0.6         | 0.8        | 0.7        | 0.6         | 0.8        | 0.7        | 0.7         | 0.8         | 0.8        | 0.7         | 0.8         |
|   | Long-term effect of reduced mature forest area | -0.8       | -0.8        | -0.9       | -0.9       | -0.8        | -1.0       | -1.0       | -0.9        | -1.1        | -1.1       | -1.0        | -1.1        |
|   | <b>Subtotal</b>                                | <b>0.1</b> | <b>-0.4</b> | <b>0.7</b> | <b>0.1</b> | <b>-0.5</b> | <b>0.7</b> | <b>0.2</b> | <b>-0.4</b> | <b>0.9</b>  | <b>0.2</b> | <b>-0.6</b> | <b>1.1</b>  |
| <b>Anthropogenic total</b>  |  | <b>5.6</b> | <b>3.6</b>  | <b>8.7</b> | <b>6.2</b> | <b>3.9</b>  | <b>9.7</b> | <b>6.7</b> | <b>4.1</b>  | <b>10.3</b> | <b>7.3</b> | <b>4.2</b>  | <b>11.4</b> |

(Tian et al., 2020)

# A comprehensive quantification of global nitrous oxide sources and sinks

- Regional N<sub>2</sub>O budgets (2007–2016)
  - Africa was the largest source of N<sub>2</sub>O in the last decade, followed by South America
  - Total anthropogenic emissions in the 10 terrestrial regions were highest in East Asia, followed by North America, Africa and Europe
- Four decades of anthropogenic N<sub>2</sub>O emissions
  - over the period 1980–2016:
    - Fluxes from Europe and Russia decreased
    - Increased: East Asia (34%), Africa (18%), South Asia (18%), South America (13%) and North America (6%)



# $\text{N}_2\text{O}$ emissions from bomas in drylands of Sub-Saharan Africa (SSA)

- Change in the source strength of abandoned bomas from 1961 to 2018

- Step 1: total livestock numbers (TLN)

- $$TLN = \sum c + \frac{(s \times 0.1 + g \times 0.1)}{0.7}$$

- c, s, g: total number of **cattle, sheep, goat**

- Step 2: boma use intensity (BUI):

- $$BUI = \frac{BAL \times NB \times FMB}{YB}$$

- BAL: **boma area per livestock**

- NB: **number of bomas** in use at the same time

- FMB: Fraction of bomas **without use of manure**

- YB: **years of boma** use

- Step 3:  $\text{N}_2\text{O}$  emission intensity ( $\text{N}_2\text{O}_{\text{int}}$ )

- $$\text{N}_2\text{O}_{\text{int}} = \text{N}_2\text{O} \times \text{N}_2\text{O}_{\text{years}} \times \frac{4}{28}$$

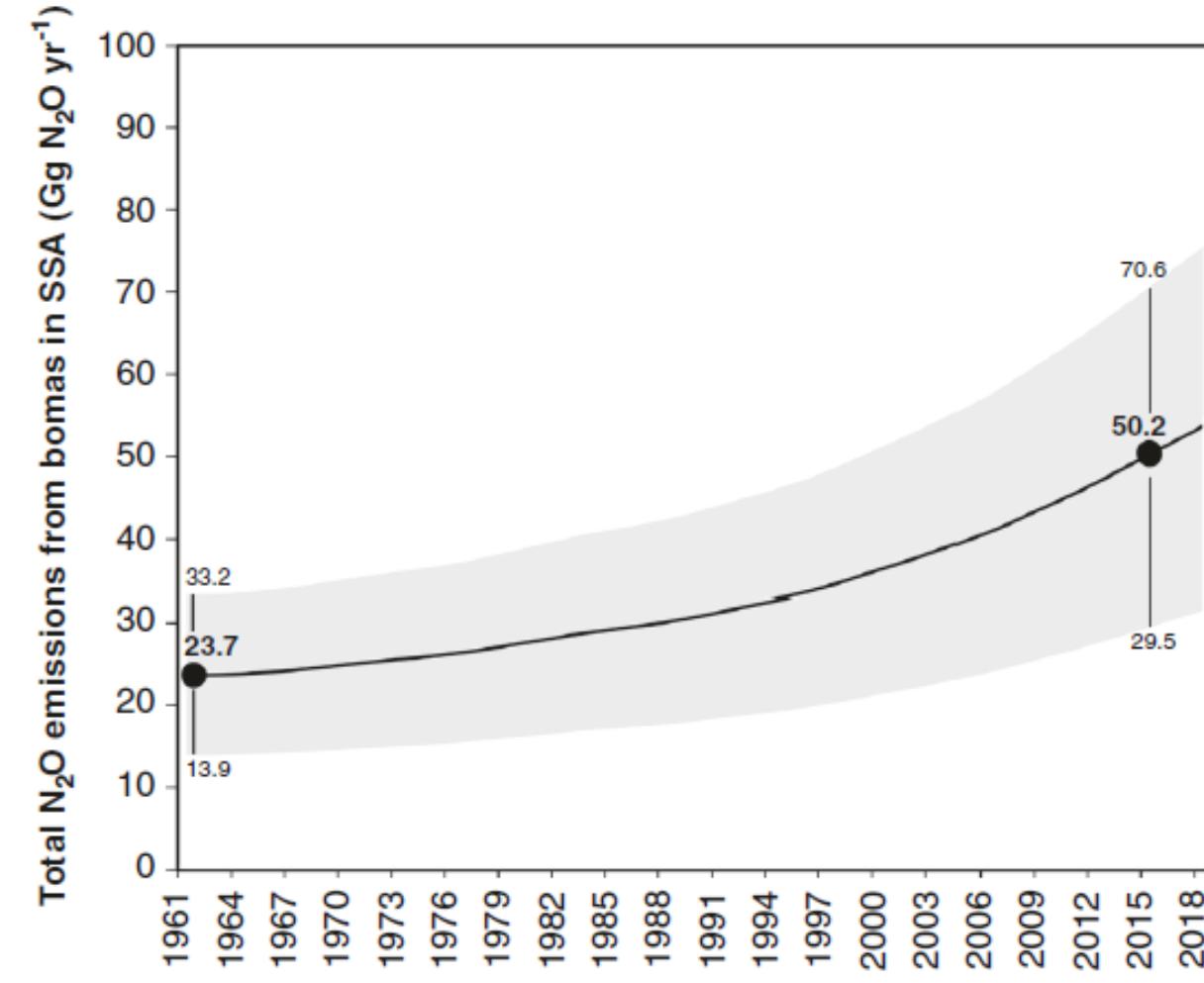
- $\text{N}_2\text{O}$ : **mean average annual  $\text{N}_2\text{O}$  flux** from bomas

- $\text{N}_2\text{O}_{\text{years}}$

- $\frac{4}{28}$ : conversion of  $\text{N}_2\text{O-N}$  to  $\text{N}_2\text{O}$

- Step 4: total  $\text{N}_2\text{O}$  emissions from bomas ( $\text{N}_2\text{O}_{\text{FB}}$ )

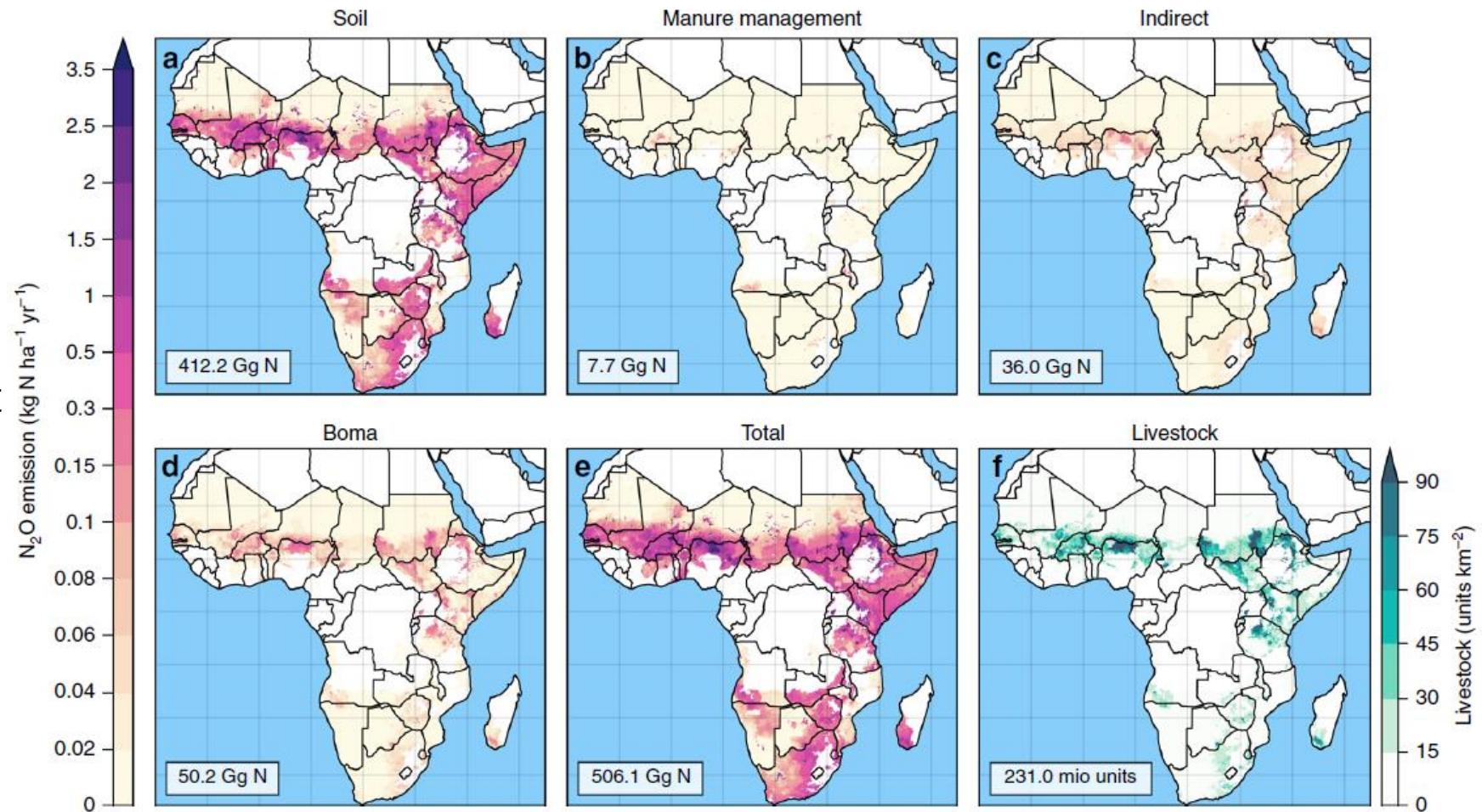
- $$\sum \text{N}_2\text{O}_{\text{FB}} = \text{TLN} \times \text{BUI} \times \text{N}_2\text{O}_{\text{int}}$$



(Butterbach-Bahl et al., 2020)

# $\text{N}_2\text{O}$ emissions from bomas in drylands of Sub-Saharan Africa (SSA)

- Sources of agricultural  $\text{N}_2\text{O}$  fluxes
  - EDGAR5
    - a: soil
    - b: manure management
    - c: indirect emission
  - in-situ measurements
    - d: total emissions from bomas (**this study**)
  - total agricultural  $\text{N}_2\text{O}$  emissions
    - e=a + b + c + d
- livestock units: livestock density
  - $N = \sum \text{cattle} + \frac{(\text{sheep} \times 0.1 + \text{goat} \times 0.1)}{0.7}$

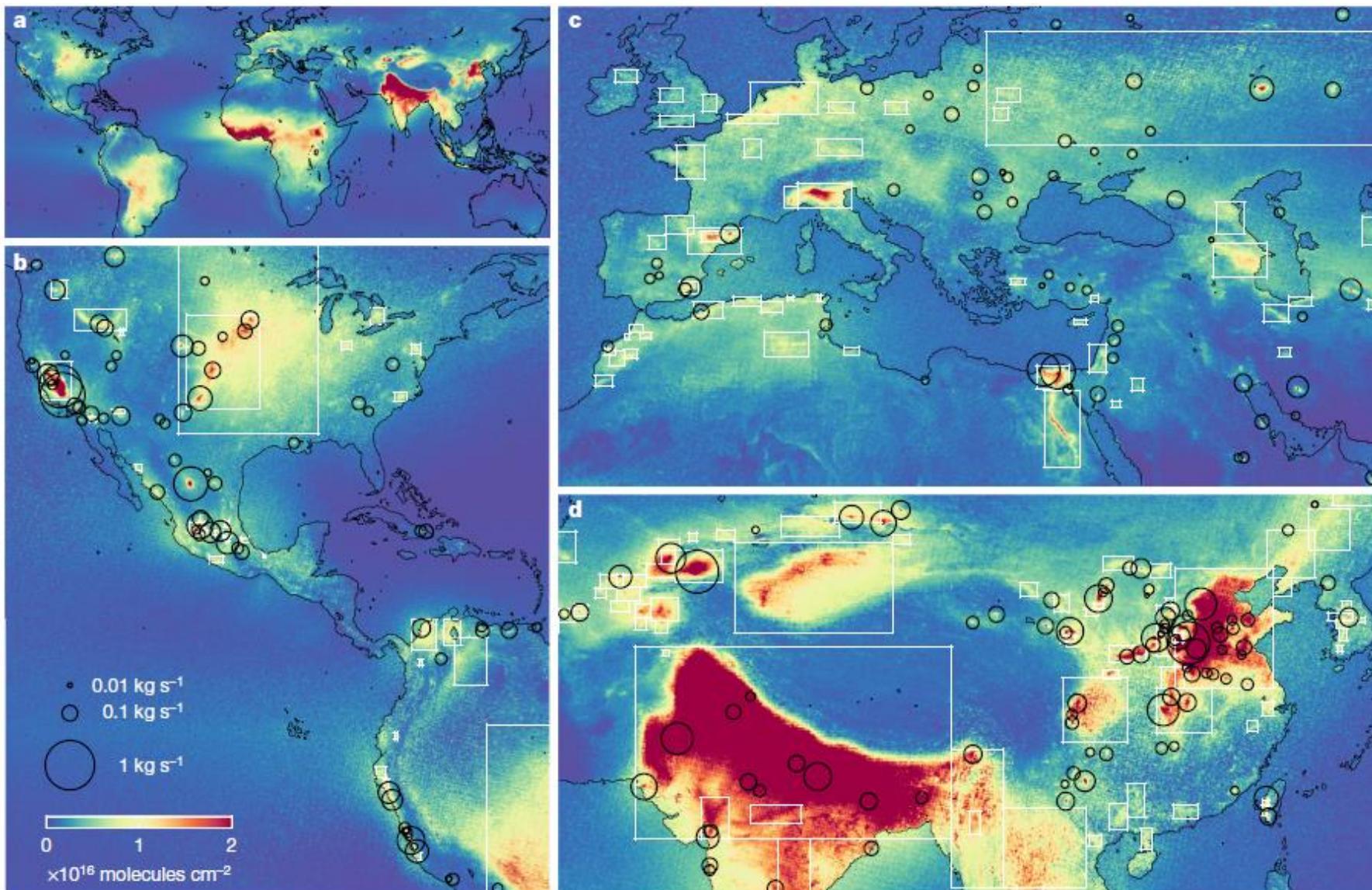


(Butterbach-Bahl et al., 2020)

# Industrial and agricultural ammonia point sources exposed

- identify, categorize and quantify **the world's ammonia emission hotspots** using a high-resolution map of atmospheric ammonia obtained from **9 years daily IASI satellite observations**.
  - Indo-Gangetic Plain
  - North China Plain
  - West Africa and Amazonia

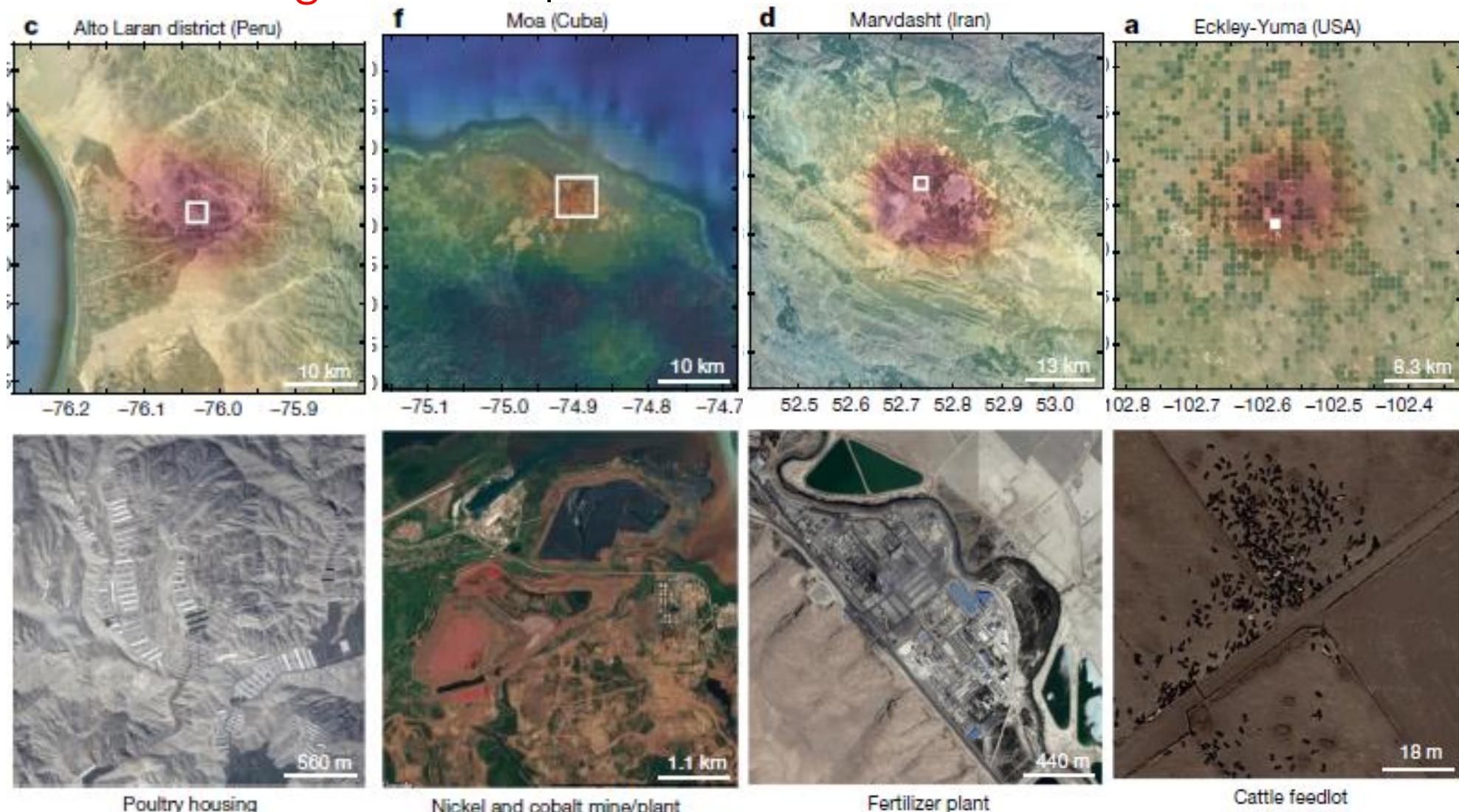
(Damme et al., 2018)



# Industrial and agricultural ammonia point sources exposed

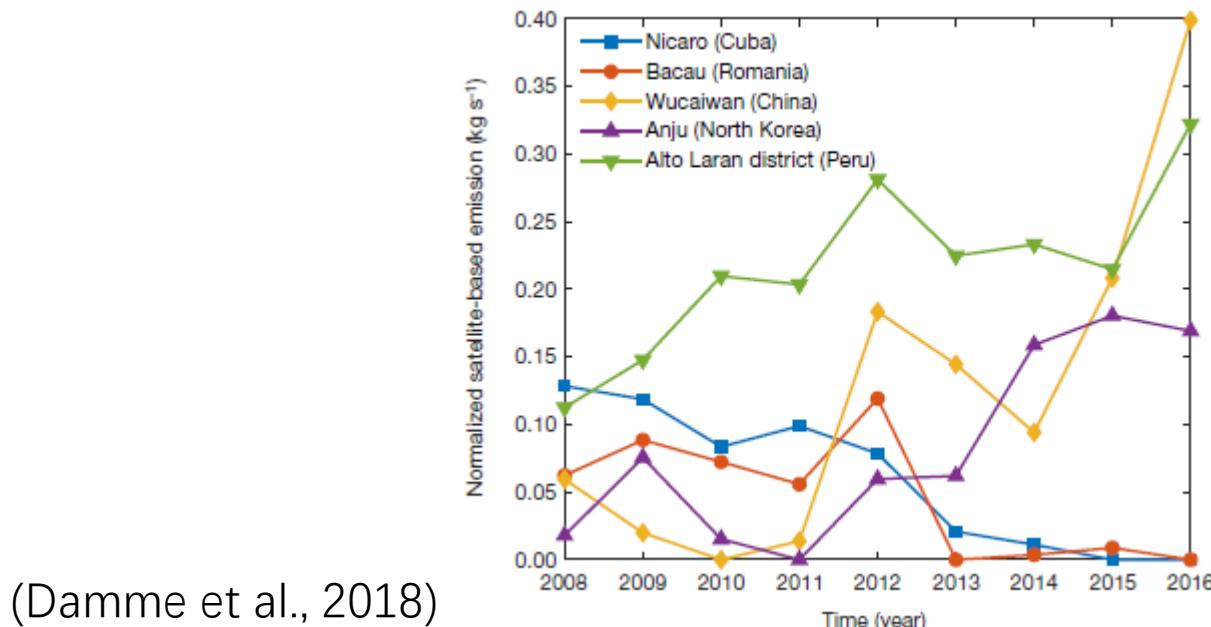
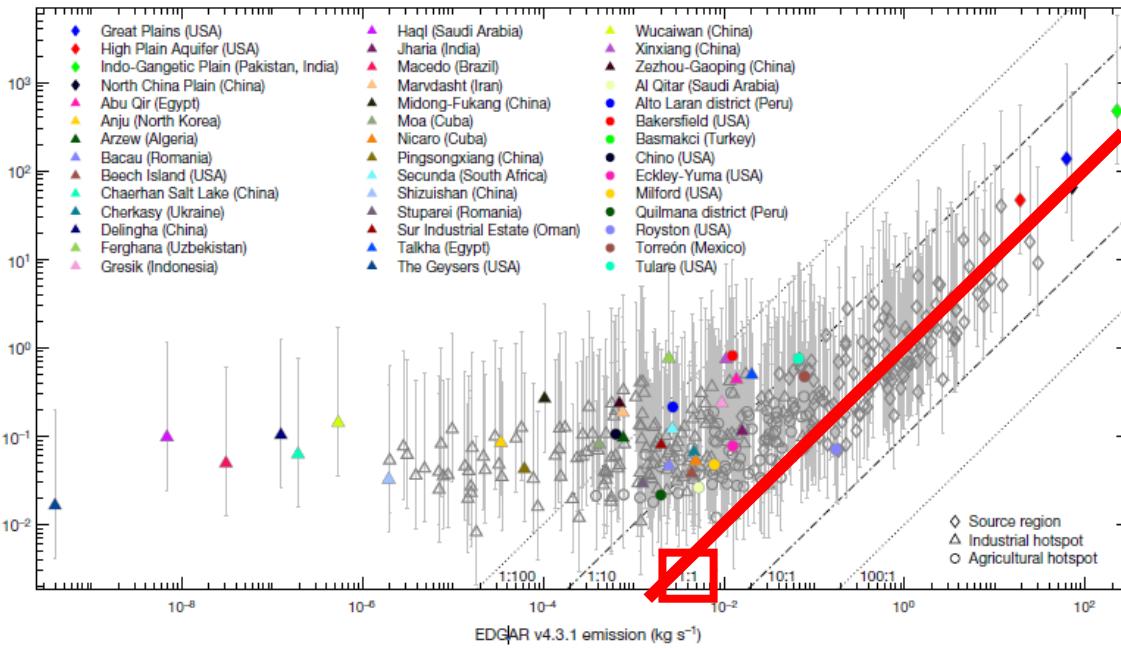
- Examples of **industrial** and **agricultural** point sources.

- agricultural
- Industrial
- natural



# Industrial and agricultural ammonia point sources exposed

- compared Satellite-derived emission with the bottom-up emission inventory EDGAR
  - emissions from almost all identified hotspots are underestimated in EDGAR
- satellite-based ammonia emission trends
  - the onset or the discontinuation of anthropogenic activity could be detected unambiguously

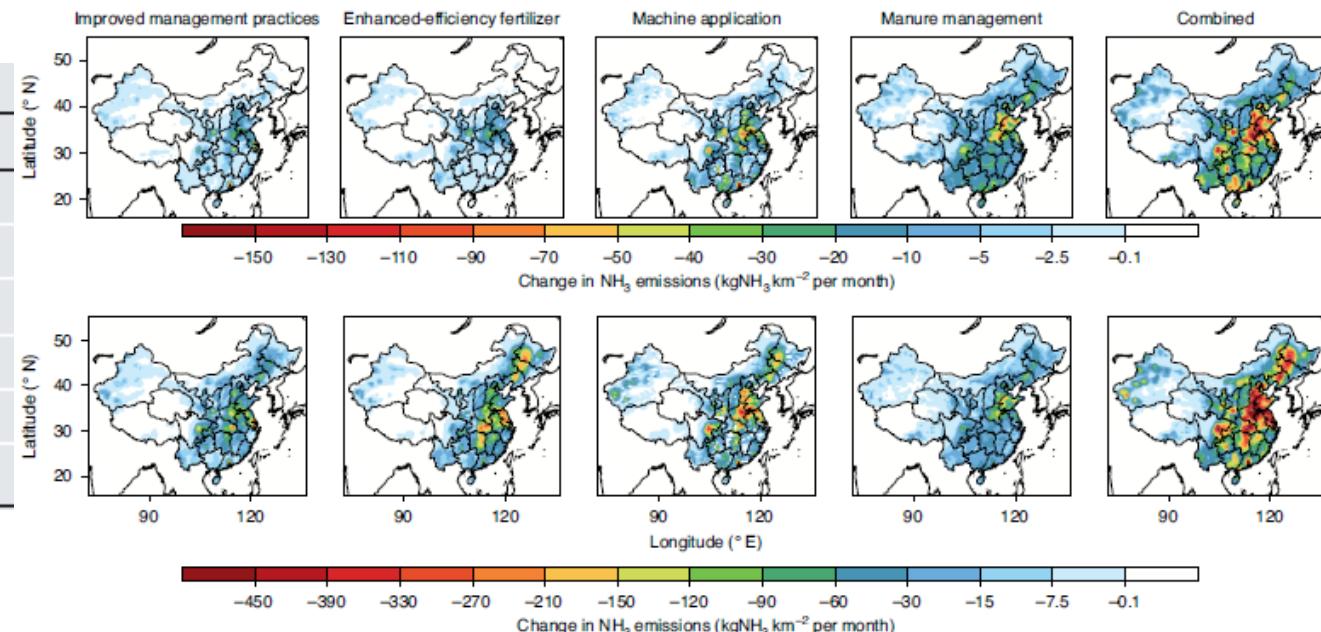


(Damme et al., 2018)

# Air quality, nitrogen use efficiency and food security in China are improved by cost-effective agricultural nitrogen management

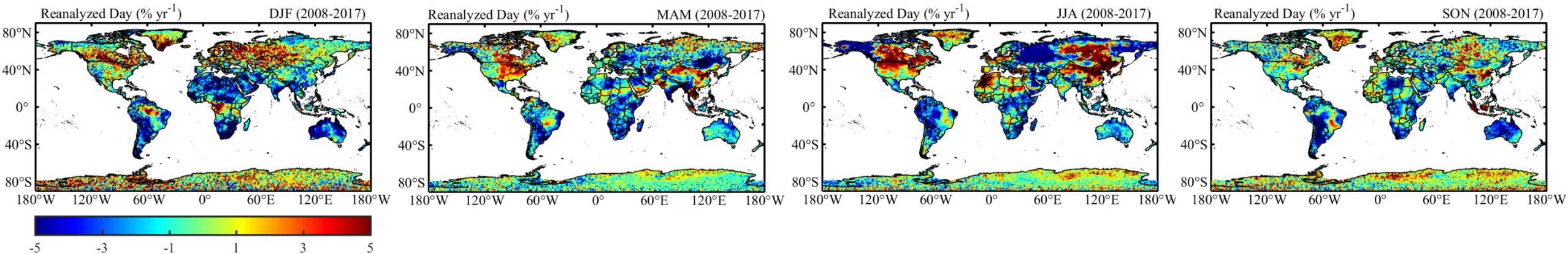
- an integrated assessment of four improved nitrogen management strategies:
  - improved farm management practices with nitrogen use reductions;
  - machine deep placement of fertilizer;
  - enhanced-efficiency fertilizer use;
  - improved manure management

| Scenario                       | NH <sub>3</sub> emissions (Tg) |         |      |
|--------------------------------|--------------------------------|---------|------|
|                                | Annual                         | January | July |
| Baseline                       | 14.0                           | 0.66    | 1.66 |
| Improved management practices  | 13.1                           | 0.64    | 1.54 |
| Enhanced-efficiency fertilizer | 12.5                           | 0.65    | 1.45 |
| Machine application            | 12.5                           | 0.62    | 1.43 |
| Manure management              | 12.5                           | 0.58    | 1.50 |
| Combined                       | 9.3                            | 0.51    | 1.01 |

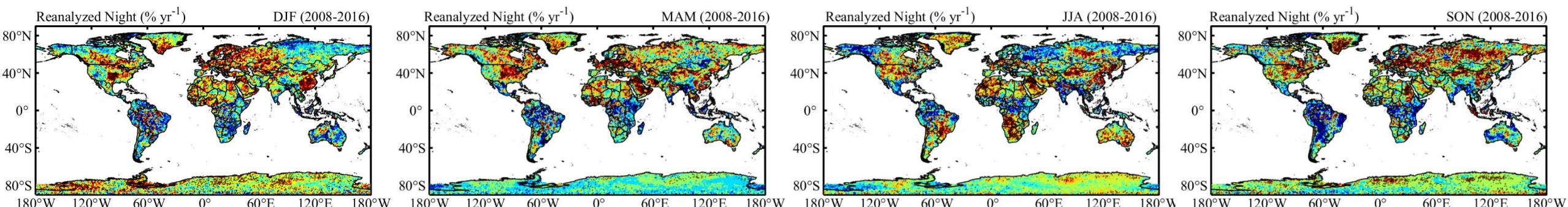


# Spatial distribution of ammonia observations trend/mean

(a) day



(b) night

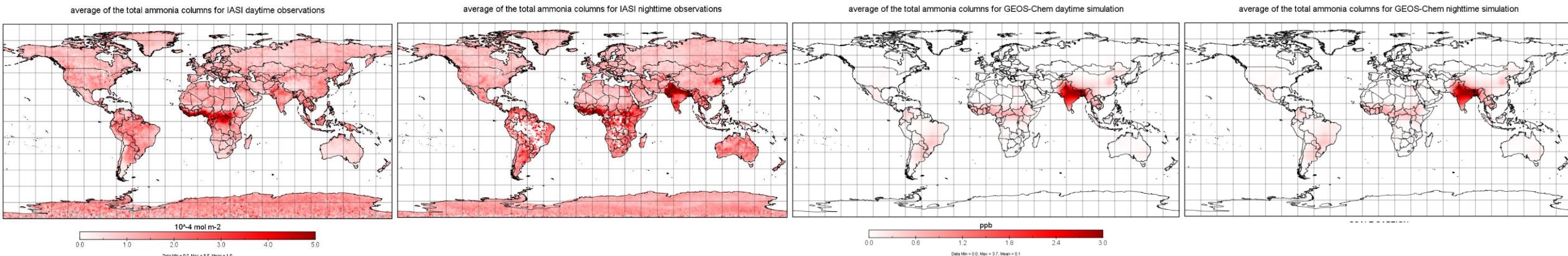


# NH<sub>3</sub> concentration from GEOS-Chem output

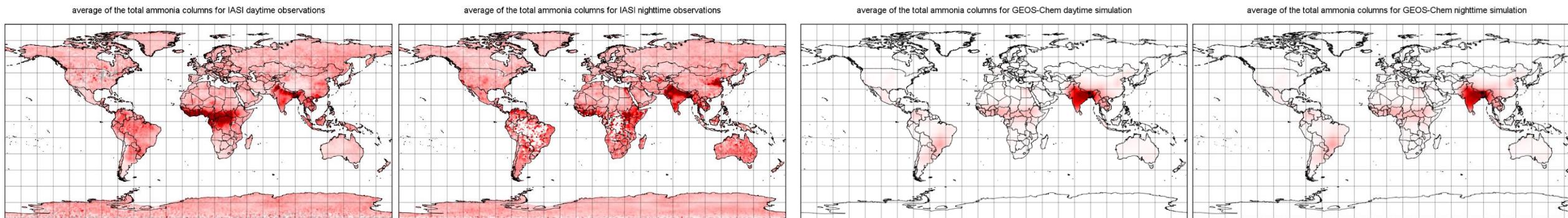
2010.1

IASI

GEOS-Chem daily



2010.2



# NH<sub>3</sub> concentration from GEOS-Chem output

2010.1

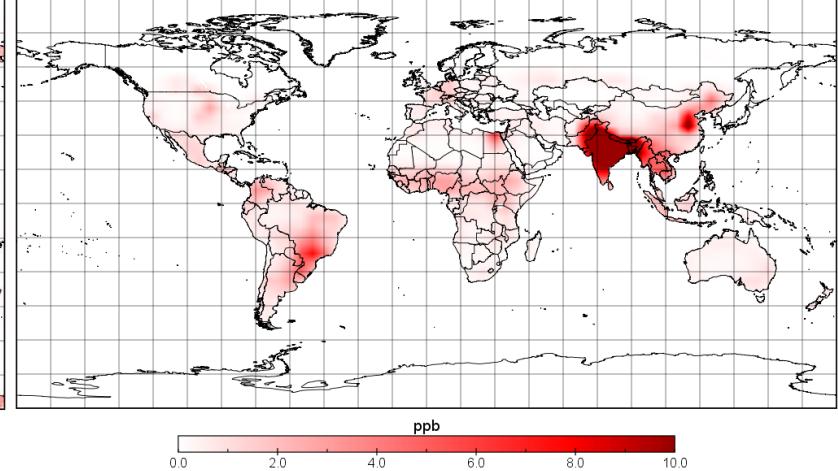
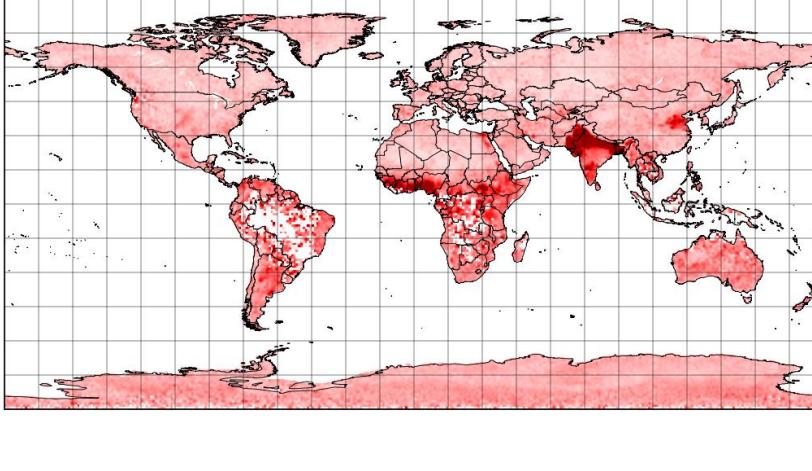
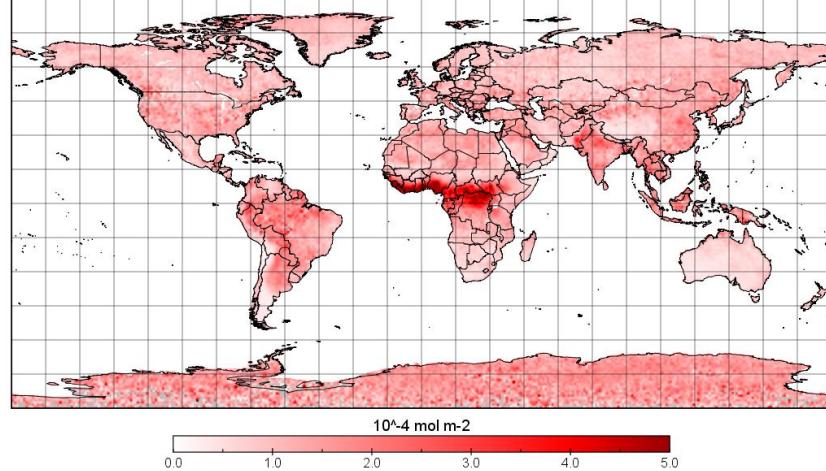
IASI

GEOS-Chem monthly

average of the total ammonia columns for IASI daytime observations

average of the total ammonia columns for IASI nighttime observations

Dry mixing ratio of species NH<sub>3</sub>

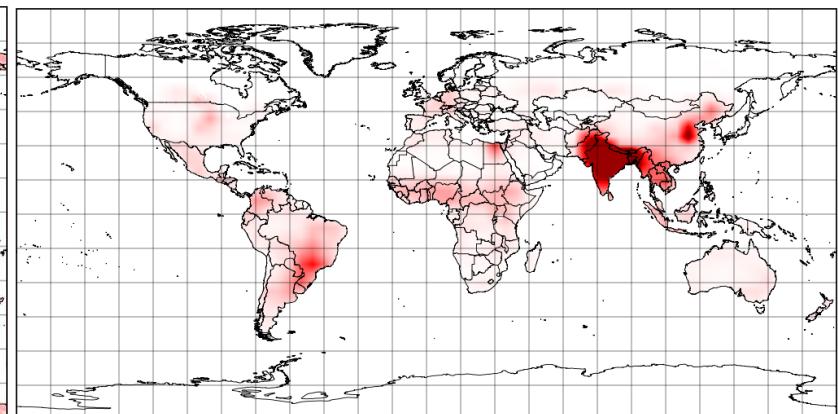
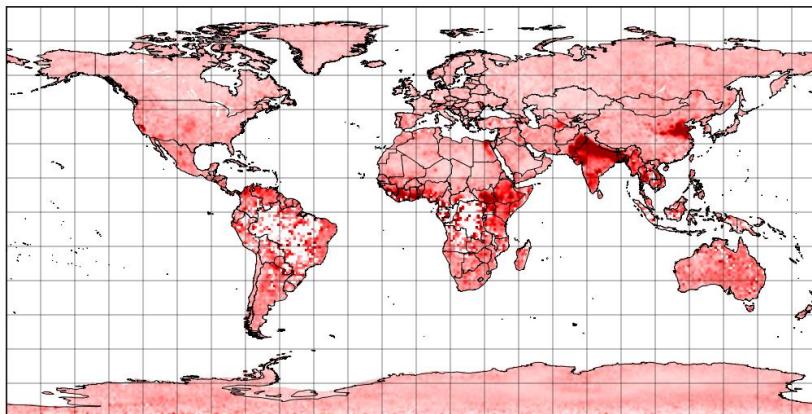
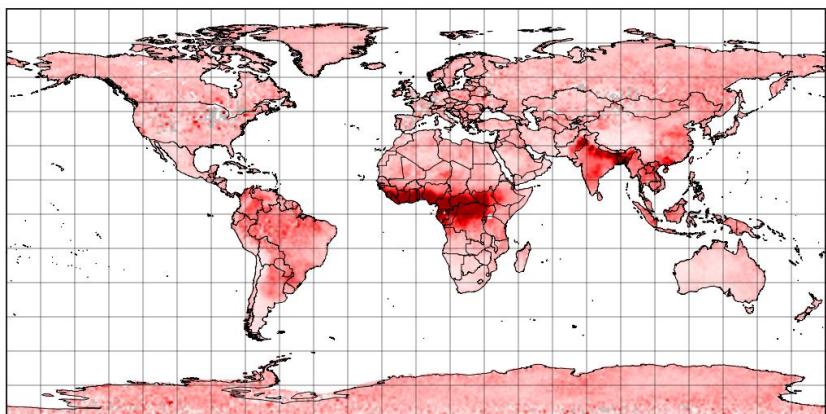


2010.2

average of the total ammonia columns for IASI daytime observations

average of the total ammonia columns for IASI nighttime observations

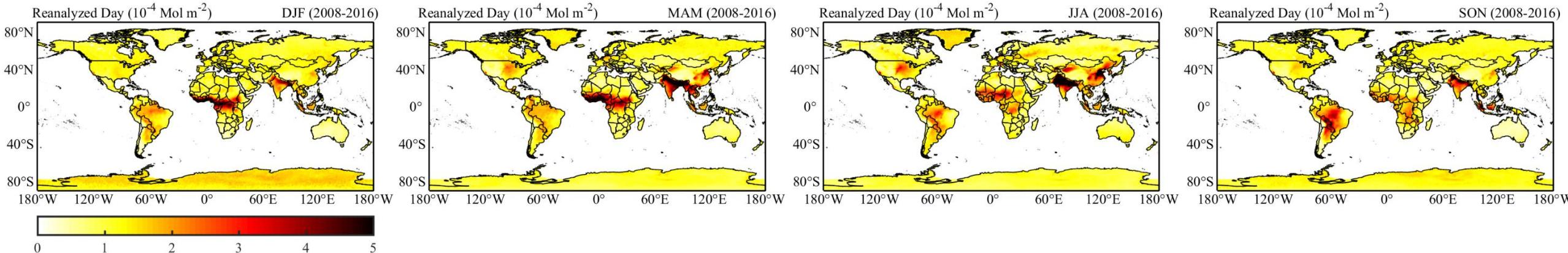
Dry mixing ratio of species NH<sub>3</sub>



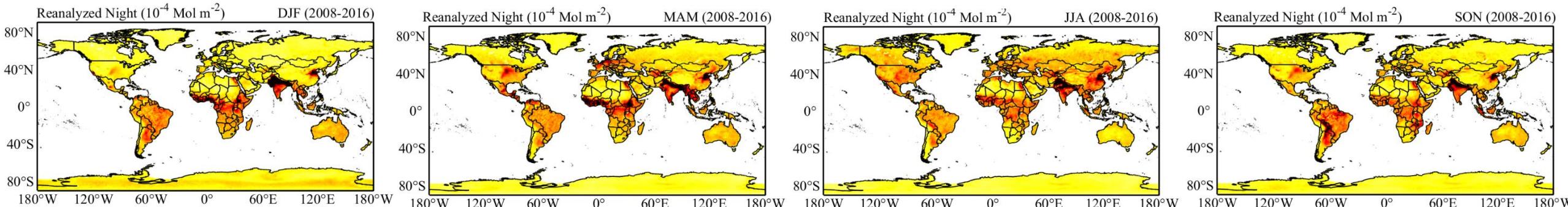


# Spatial distribution of ammonia observations mean

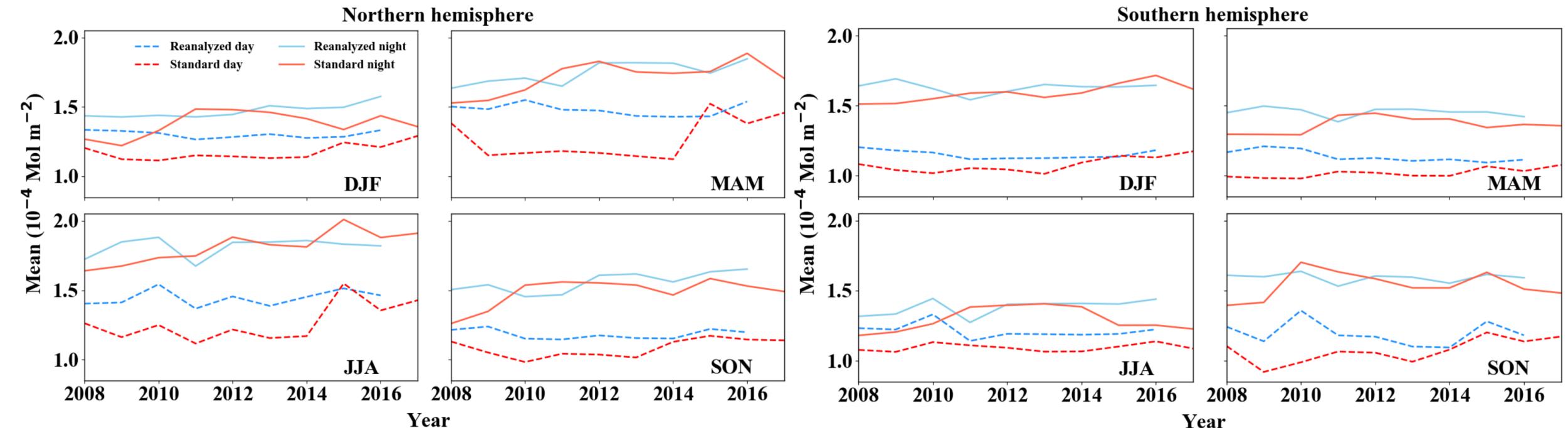
(a) day



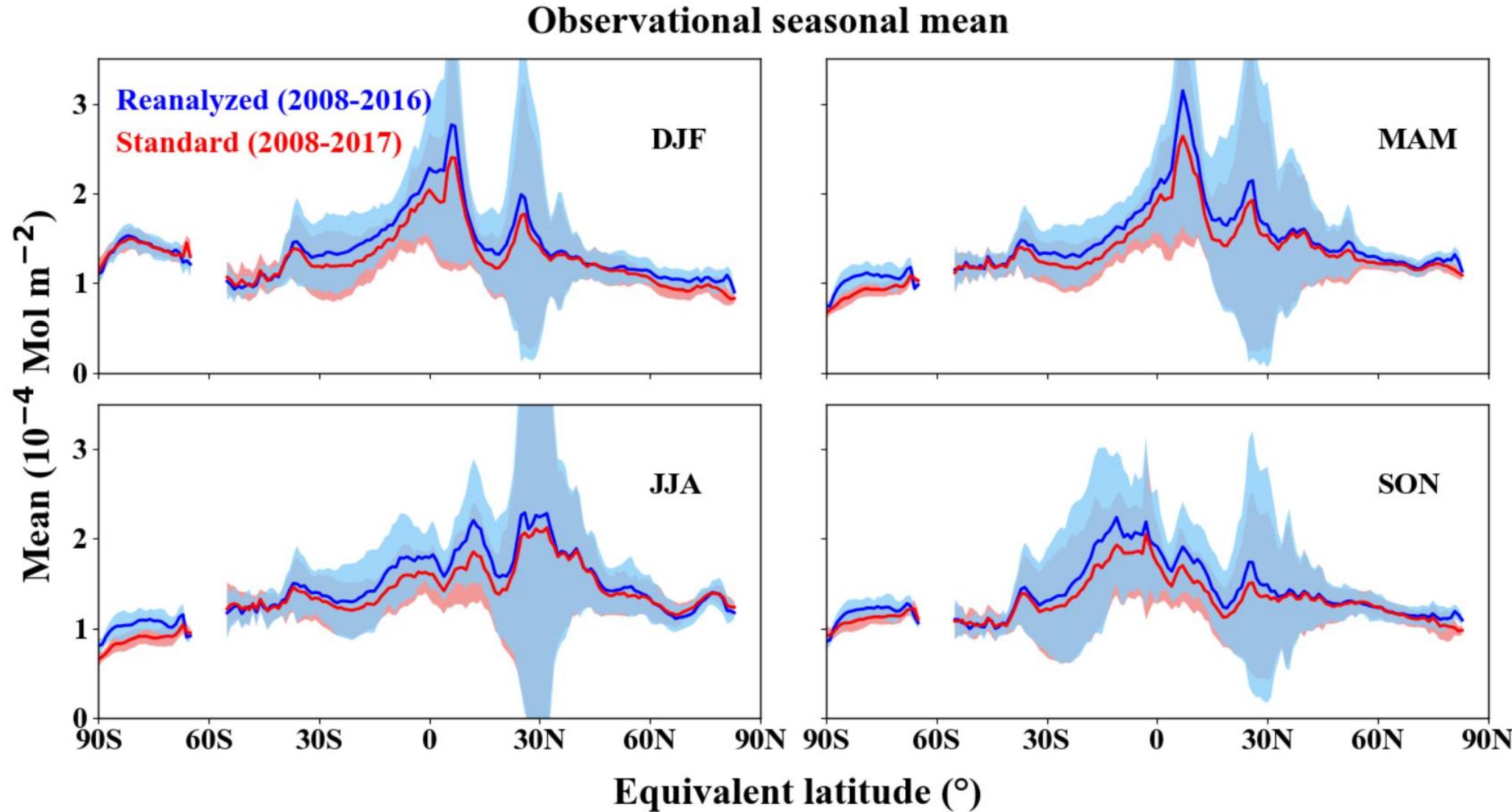
(b) night



# Seasonal change for NH and SH (day and night)

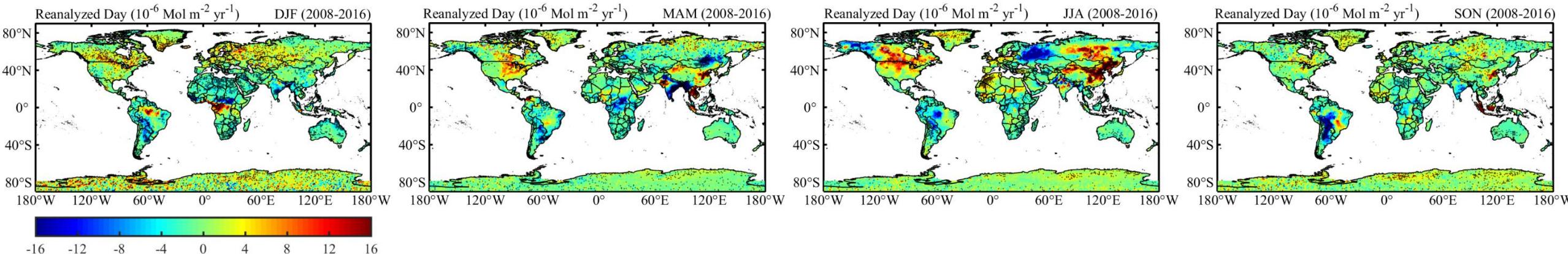


# Seasonal mean of Land for equivalent latitude (within 1 sigma standard deviations)

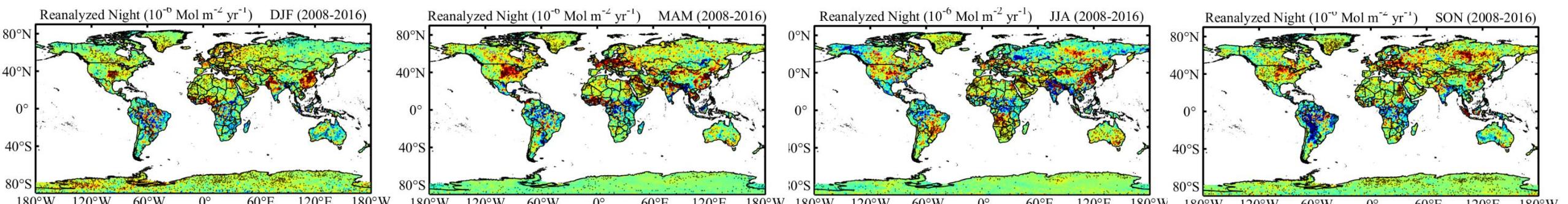


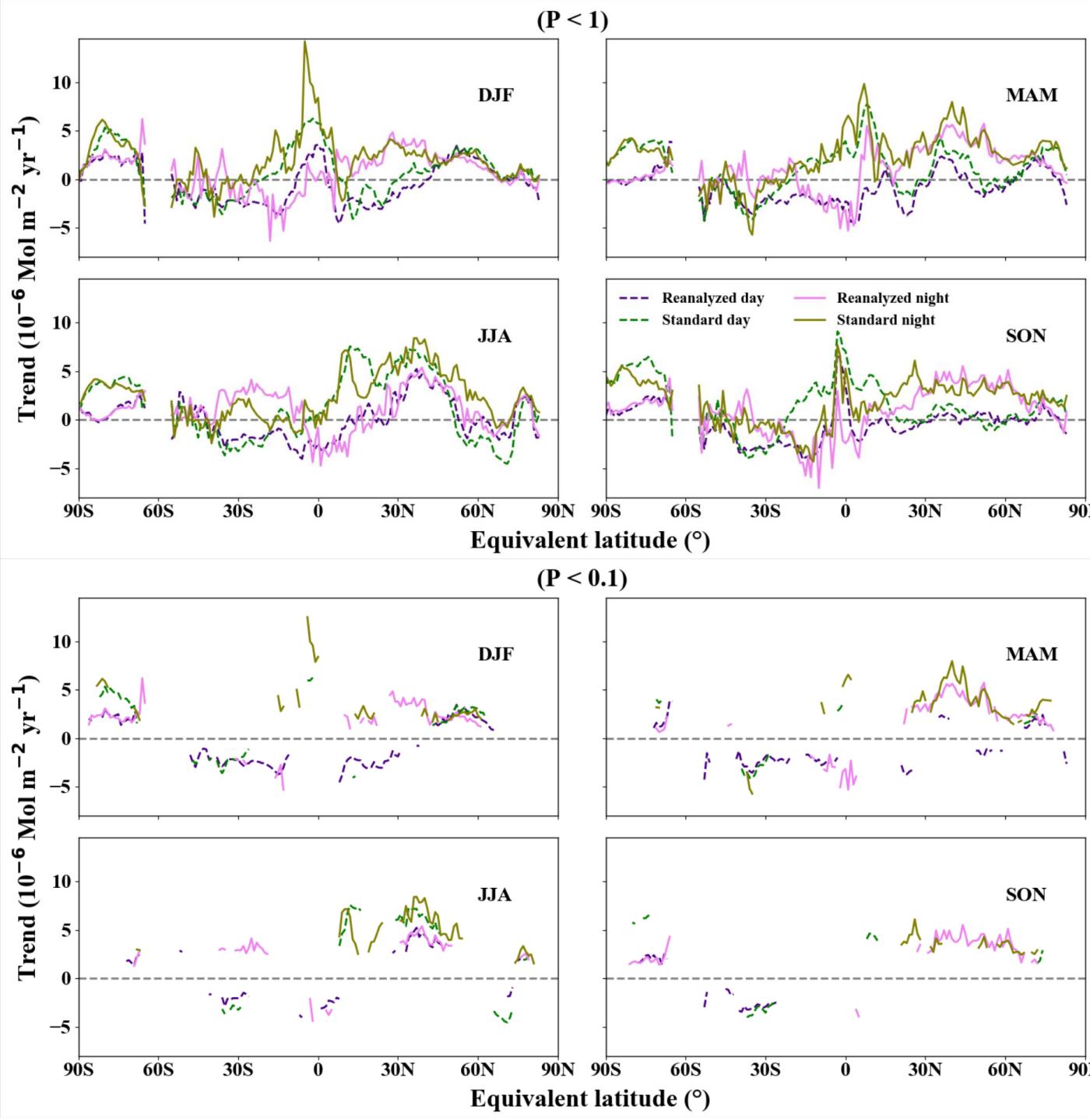
# Spatial distribution of ammonia observations trend

(a) day



(b) night

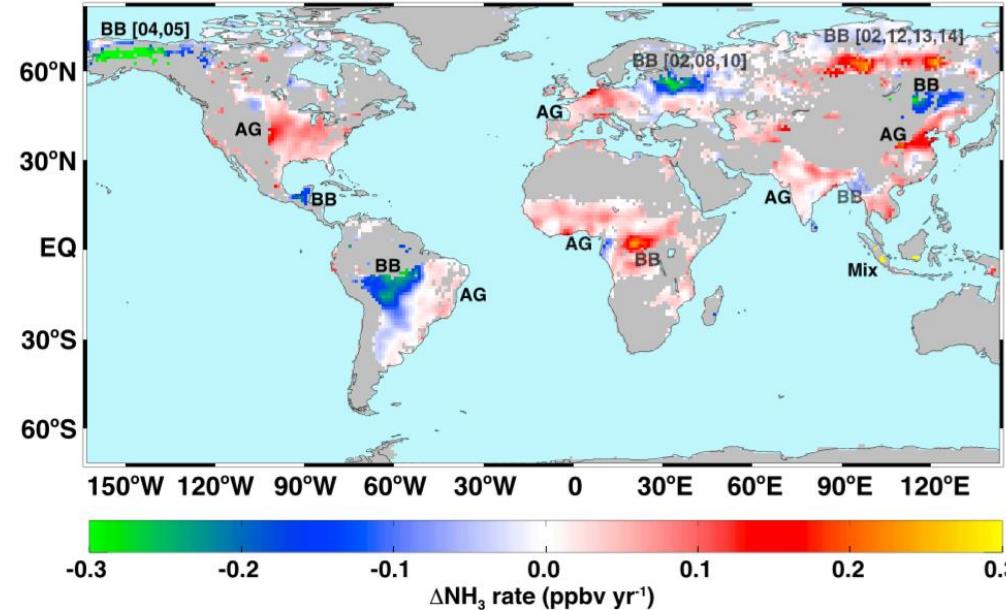




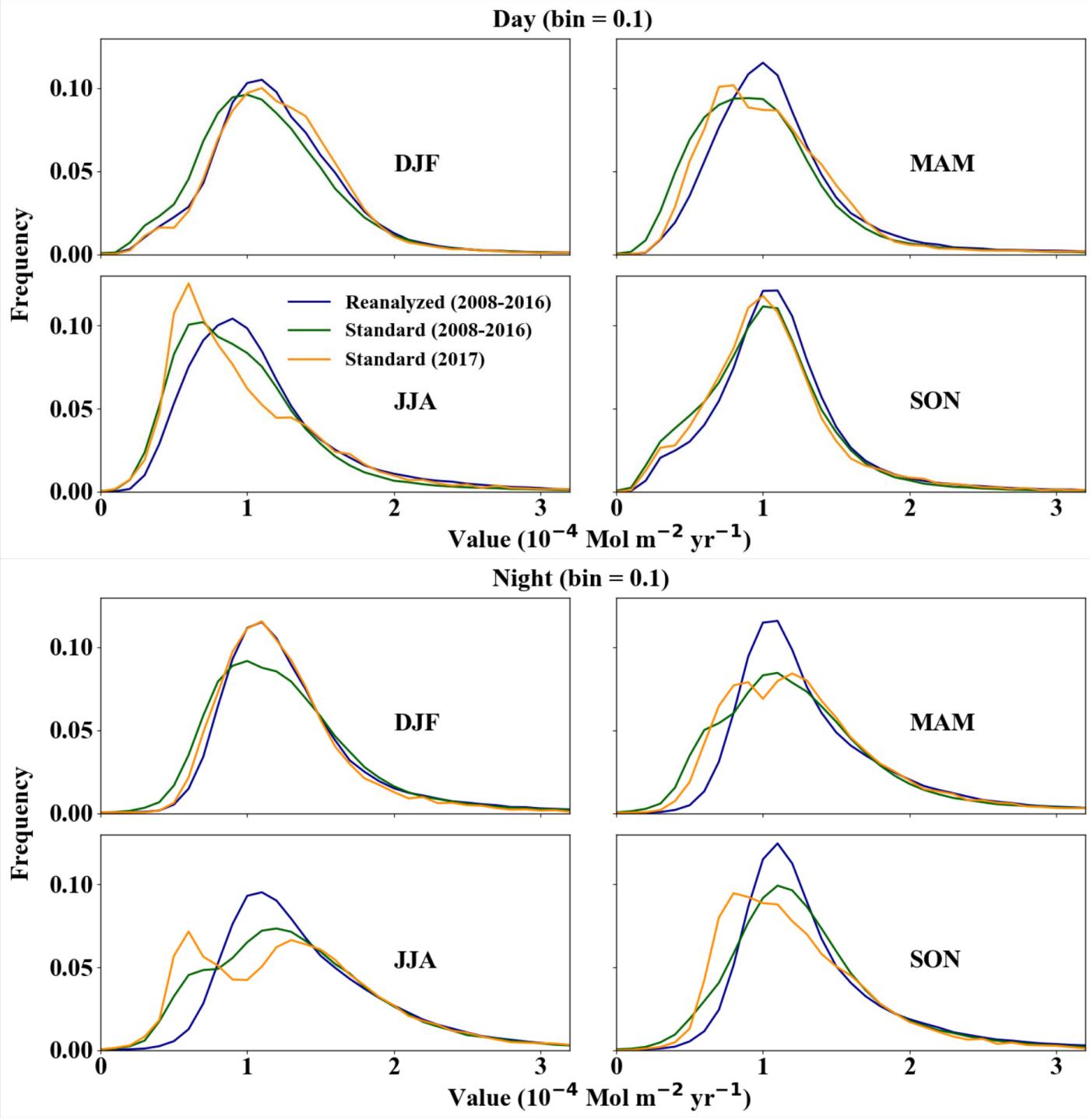
Seasonal trend in the equivalent latitude over 2008-2016 (day and night)

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

- provides evidence of substantial increases in atmospheric ammonia (NH<sub>3</sub>) concentrations (14 year) over several of the world's major agricultural regions
- The rate of change of NH<sub>3</sub> volume mixing ratio (VMR) in parts-per-billion by volume (ppbv) per year computed
  - BB: biomass burning
  - AG: agricultural

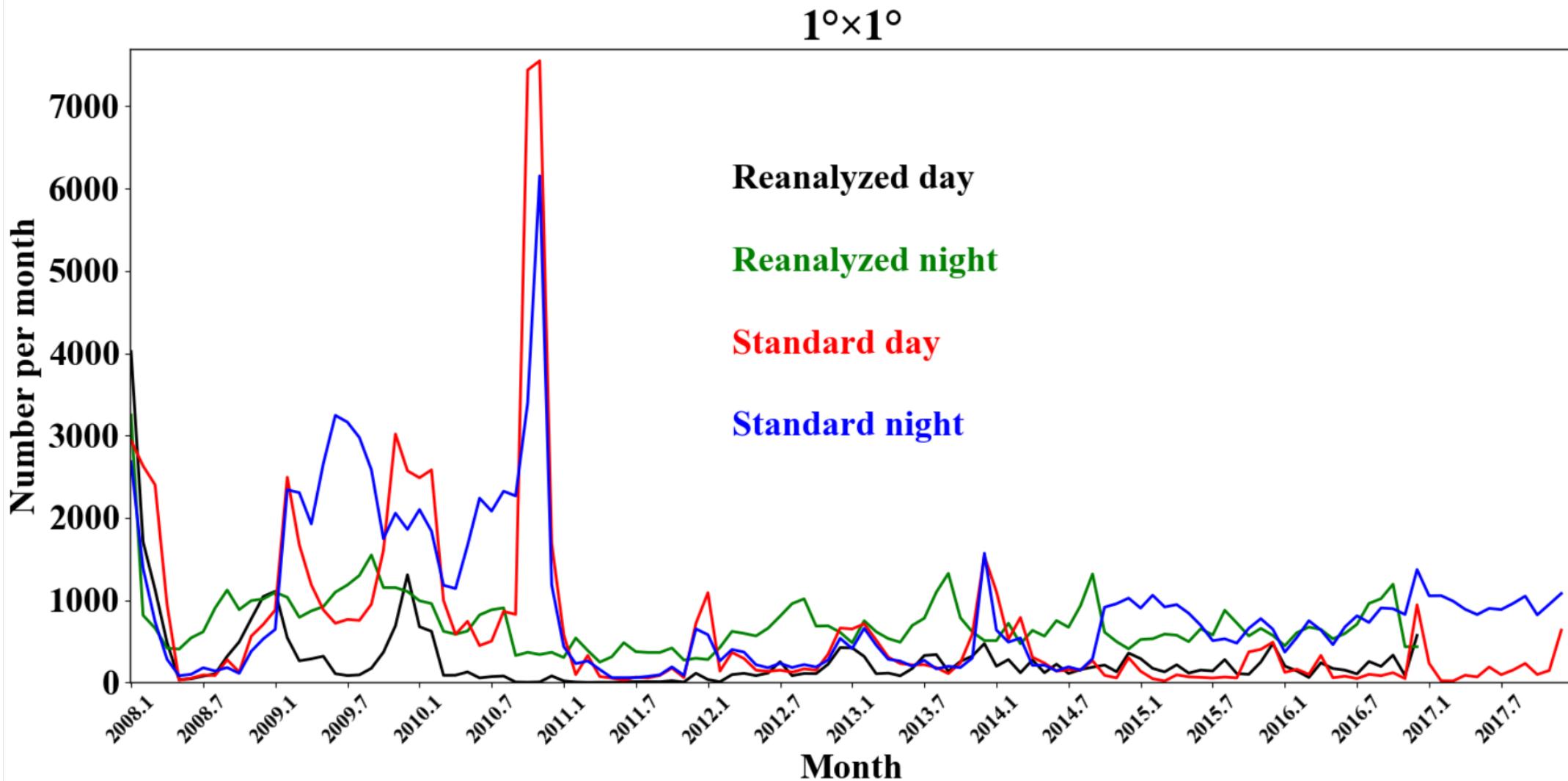


(Warner et al, 2016)



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

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



End

# 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 used
    - GEOS-Chem horizontal grid
    - GEOS-Chem simulation item
    - Starting time
    - Ending time
- 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

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

# 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"
      - 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

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) |

# GEOS-Chem simulation

- Output files
  - Log files
    - compile.log: echo-back of the GEOS-Chem compilation output
    - lastbuild: a summary of all of the options that were used to build the GEOS-Chem executable
    - GC\_\*.log: an "echo-back" of all input options that were specified in input.geos,
      - the list of diagnostic quantities that are being archived
      - the list of files that are being read
      - information about the operations that are being done at each GEOS-Chem timestep
    - log.dryrun: the full path names of all input that are read by GEOS-Chem.
    - HEMCO.log: information about how emissions, met fields, and other relevant data are read from disk and processed by HEMCO for input into GEOS-Chem
    - slurm-JOBID.out: used a batch scheduler such as SLURM, PBS, LSF, etc. to submit your GEOS-Chem simulation
  - Restart files
    - GEOSChem.Restart.YYYYMMDD\_hhmmz.nc4: species concentrations that are read in at simulation startup
    - HEMCO\_restart.YYYYMMDDhhmm.nc: save out certain quantities in order to facilitate long GEOS-Chem simulations with several run stages
  - Diagnostic output files

# GEOS-Chem simulation

- Output files
  - Log files
    - compile.log: echo-back of the GEOS-Chem compilation output
    - lastbuild: a summary of all of the options that were used to build the GEOS-Chem executable
    - GC\_\*.log: an "echo-back" of all input options that were specified in input.geos,
      - the list of diagnostic quantities that are being archived
      - the list of files that are being read
      - information about the operations that are being done at each GEOS-Chem timestep
    - log.dryrun: the full path names of all input that are read by GEOS-Chem.
    - HEMCO.log: information about how emissions, met fields, and other relevant data are read from disk and processed by HEMCO for input into GEOS-Chem
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  - Diagnostic output files

# Error fixed by Dr. Zhang

```
Set HEMCO clock to 2010-01-31 06:40:00
The weekday is (0=Sun,...,6=Sat): 0
Is this an emission time step : T

Now reading always list!
HEMCO emissions successfully calculated!
Calculate air-sea flux for HEMCO species 40
Module species name: DMS
Calculate air-sea flux for HEMCO species 1
Module species name: ACET
Calculate air-sea flux for HEMCO species 122
Module species name: MOH
Calculate air-sea flux for HEMCO species 4
Module species name: ALD2
Calculate air-sea flux for HEMCO species 120
Module species name: MENO3
Calculate air-sea flux for HEMCO species 47
Module species name: ETNO3
HEMCO emissions successfully calculated!
```

```
forrtl: error (65): floating invalid
Image          PC            Routine      Line      Source
libintlc.so.5  00002AB4F8A9F961 Unknown
libintlc.so.5  00002AB4F8A9E0B7 Unknown
libnetcdff.so.7 00002AB4F668D432 Unknown
libnetcdff.so.7 00002AB4F668D286 Unknown
libnetcdff.so.7 00002AB4F6673E2C Unknown
libnetcdff.so.7 00002AB4F6678172 Unknown
libpthread.so.0 00000035E7C0F130 Unknown
geos           0000000001C8F65E gckpp_hetrates_mp    503  gckpp_HetRates.F90
geos           00000000009204A2 flexchem_mod_mp_d   801  flexchem_mod.F90
libiomp5.so    00002AB4F87F6BB3 Unknown
libiomp5.so    00002AB4F87CB617 Unknown
libiomp5.so    00002AB4F87CAD3A Unknown
libiomp5.so    00002AB4F87F6EAD Unknown
libpthread.so.0 00000035E7C07DF3 Unknown
libc.so.6       00000035E78F62CD Unknown
/home/jointforce/default/spool/ibnode135/job_scripts/851352: line 25: 22528 Aborted
```

```
--> DATE: 2010/01/31 UTC: 06:30 X-HRS: 726.500000
    - DIAG51: Accumulation at 2010/01/31 06:40
    - DIAG51b: Accumulation at 2010/01/31 06:40
--> DATE: 2010/01/31 UTC: 06:40 X-HRS: 726.666687
```



# Nitrogen-containing compounds

- Nitrous oxide (N<sub>2</sub>O): an extremely potent greenhouse gas
  - Source: **tropical soil**, biomass burning, degassing of irrigation water, agricultural activities, industrial processes, **ocean**
  - Sink: photodissociation in the stratosphere (90%), reaction with excited oxygen atoms (10%)

TABLE 2.5 Global N<sub>2</sub>O Budget (Tg N yr<sup>-1</sup>) for 2006

| Anthropogenic sources                         |      |
|---|------|
| Fossil fuel combustion and industrial sources | 0.7  |
| Agriculture                                   | 4.1  |
| Biomass and biofuel burning                   | 0.7  |
| Human excreta                                 | 0.2  |
| Other   | 0.6  |
| Total anthropogenic sources                   | 6.9  |
| Natural sources                               |      |
| Soils   | 6.6  |
| Oceans  | 3.8  |
| Atmospheric chemistry                         | 0.6  |
| Total natural sources                         | 11.0 |
| Total natural + anthropogenic sources         | 17.9 |
| Stratospheric sink (see Chapter 5)            | 14.3 |
| Observed growth rate                          | 3.6  |

Source: IPCC (2013).

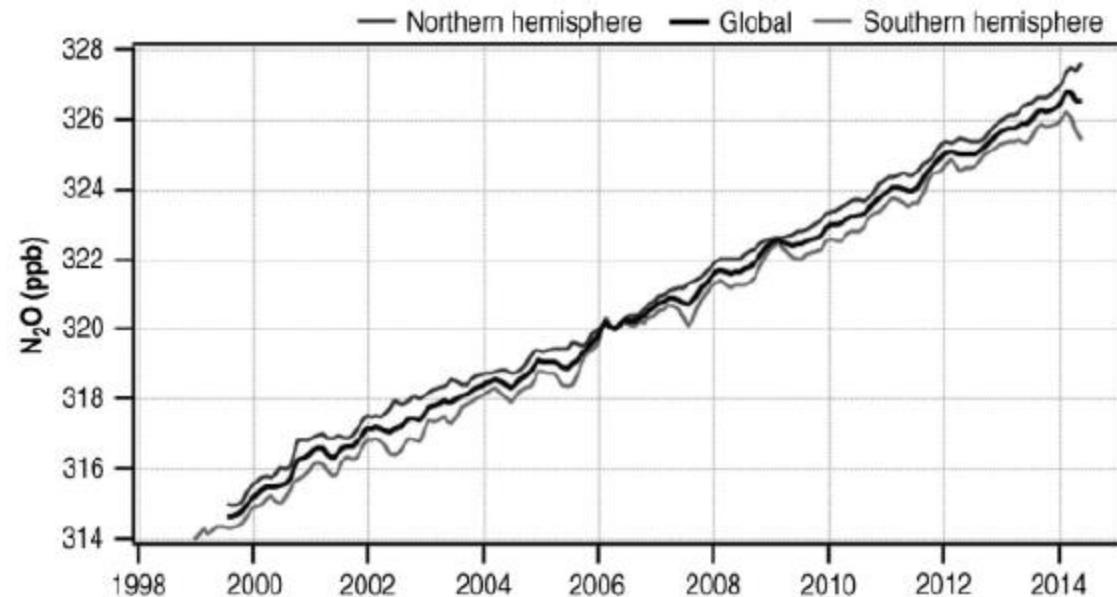


FIGURE 2.3 Global atmospheric mixing ratio of N<sub>2</sub>O from 1999 through 2013 (Source: NOAA/ESRL; available at [www.esrl.noaa.gov/gmd/hats/insitu/cats/conc/mlon20.html.](http://www.esrl.noaa.gov/gmd/hats/insitu/cats/conc/mlon20.html.))

# Nitrogen-containing compounds

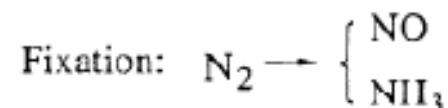
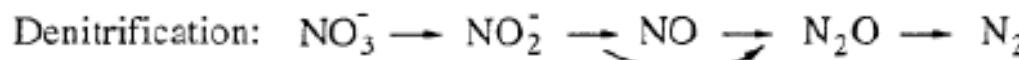
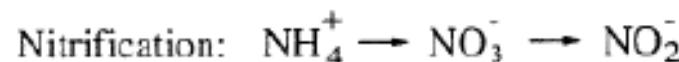
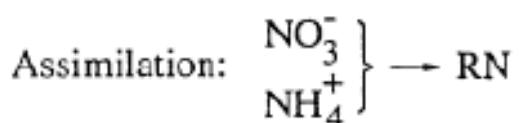
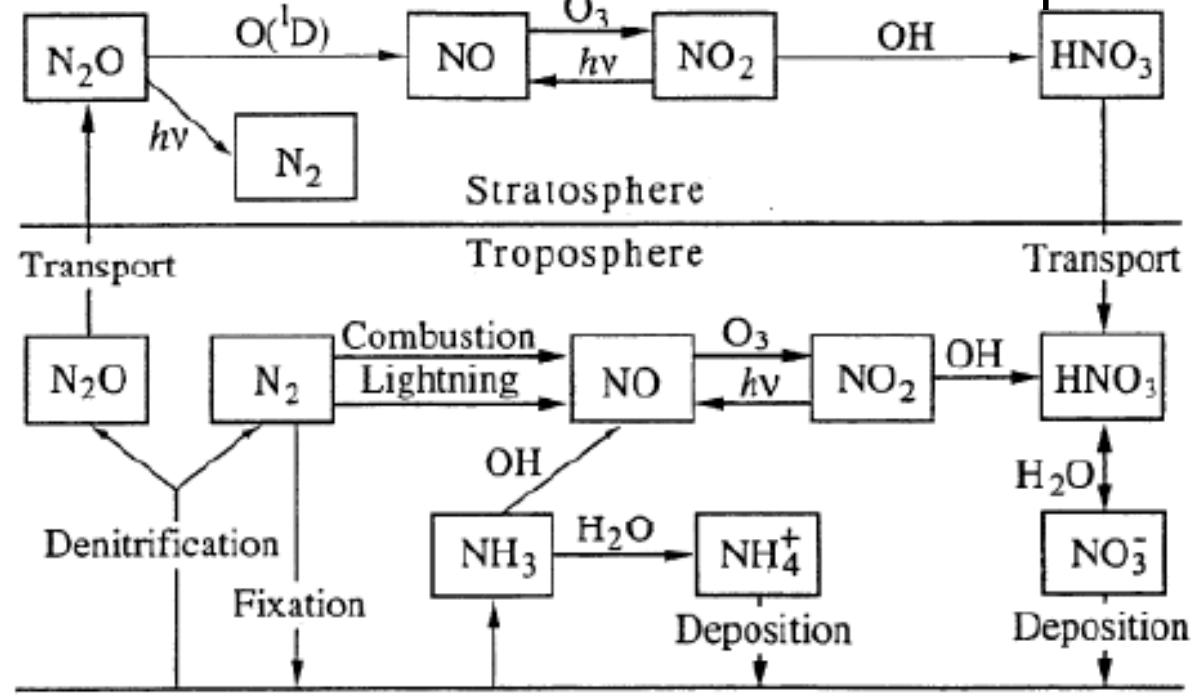
- Nitrogen Oxide ( $\text{NO}_x \equiv \text{NO} + \text{NO}_2$ )
- Reactive odd nitrogen ( $\text{NO}_y$ ): major in urban-suburban areas
- **Ammonia** ( $\text{NH}_3$ ): the most abundant nitrogen-containing compound
  - Source: animal waste, ammonification of humus from soils, losses of fertilizers from soils, industrial
  - Residence time: 10 days
- Amines: organic

**TABLE 2.8 Estimated Annual Global Ammonia Emissions**

| Source  | Amount (Tg N yr <sup>-1</sup> ) |
|---|---------------------------------|
| Agricultural (domestic animals, synthetic fertilizers, crops) | 37.4                            |
| Natural (oceans, undisturbed soils, wild animals)             | 10.7                            |
| Biomass burning   | 6.4                             |
| Other (humans and pets, industrial processes, fossil fuels)   | 3.1                             |
| Total   | 57.6                            |

Source: Bouwman et al. (1997).

# Nitrogen compounds processes in the atmospheric cycle



# Nitrogen Oxide Radicals ( $\text{NO}_x \equiv \text{NO} + \text{NO}_2$ )

- The largest source is combustion:
  - thermal Nox (2000K):  $\text{N}_2 + \text{O} \rightarrow \text{NO} + \text{N}$ ,  $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$
  - fuel Nox (low flame temperatures)
- the main source of Nox in stratosphere:
  - $\text{O} (1\text{D}) + \text{N}_2\text{O} \rightarrow \text{NO} + \text{NO}$
- A dominant sink for NO in both the troposphere and stratosphere:
  - null cycle:  $\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$        $\text{NO}_2 + h\nu (\lambda < 400 \text{ nm}) \xrightarrow{\text{O}_2} \text{NO} + \text{O}_3$
- Alternate reaction cycles for NO and NO<sub>2</sub>:
  - rate-limiting step for ozone loss:  $\text{NO}_2 + \text{O} \rightarrow \text{NO} + \text{O}_2$
- Loss of Nox:
  - Daytime:  $\text{NO}_2 + \text{OH} + \text{M} \rightarrow \text{HNO}_3 + \text{M}$
  - Night:  $\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$ ,  $\text{NO}_2 + \text{NO}_3 + \text{M} \rightarrow \text{N}_2\text{O}_5 + \text{M}$     $\text{N}_2\text{O}_5 + \text{H}_2\text{O} \xrightarrow{\text{aerosol}} 2\text{HNO}_3$