Ammonia concentrations emissions from observation and modeling simulation 5

IASI satellite and GEOS-Chem model

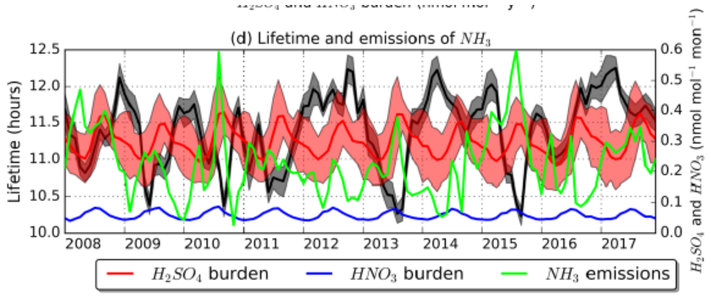
2021.1

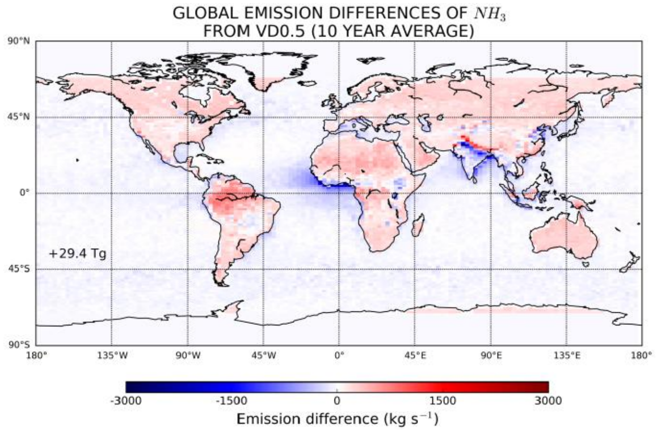
- Accomplished:
  - 1. literature: global NH_3 emissions over 2008-2017
  - 2. literature: Industrial and agricultural ammonia point sources exposed (second time)
  - 3. keep negative value in the IASI daily data (filter: cloud coverage < 10%, skin temperature > 263.15K)
  - 4. calculate IASI emissions based on effective lifetime from GEOS-Chem
  - 5. wet deposition, dry deposition and transport of NH_3/NH_4^+ from GEOS-Chem
  - 6. filter the IASI concentration again by the mean number of retrievals
- Ammonia/ammonium Data:
  - IASI total columns: Reanalyzed IASI/Metop-A
    - Daily, L2, 1°×1° (2008-2018)
  - GEOS-Chem simulation, 4°×5°, daily, 2008-2018
    - Total column concentration
    - Total column transport/chemistry/deposition rate of change
    - Total column emissions
- Meteorological input data
  - ECMWF ERA5 skin temperature, 0.25°x0.25°
    - hourly data on single levels (2008-2018), 9:00/10:00

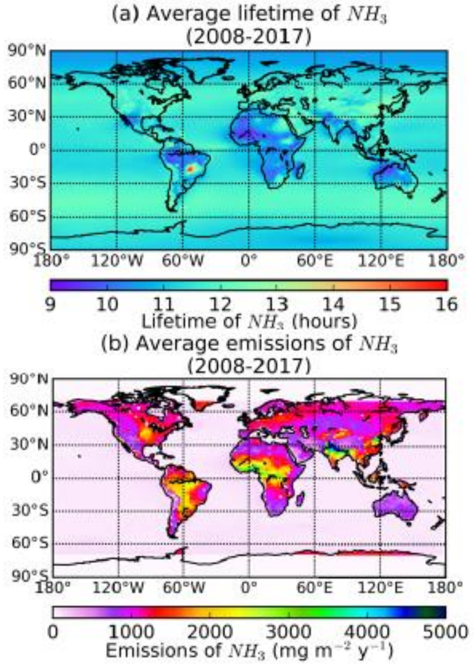
literature

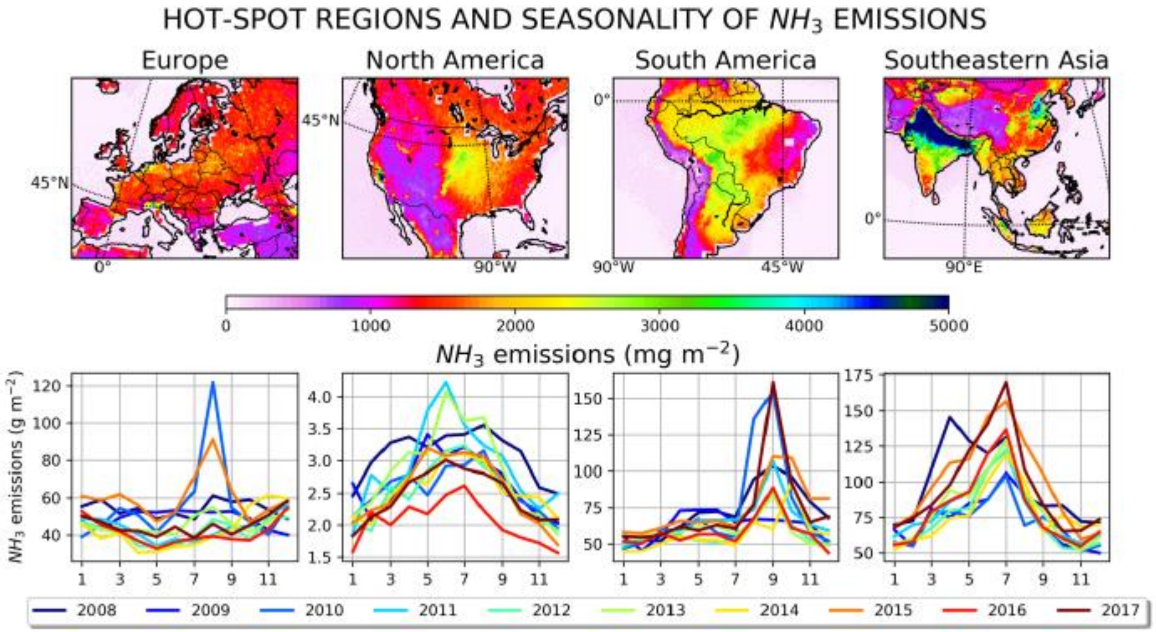
Global NH3 emissions (2008-2017)

- NH3 implications:
  - Population: formation of PM2.5
  - Environment: ecosystems
  - Climate impact: radiative balance
- Data:
  - Monitoring:
    - EMEP (Europe)
    - EAAD (Southeastern Asia)
    - AMoN-US (US)
    - NAPS (Canda)
  - Satellite:
    - IASI: ANNI NH3-v2.1R-I product
    - CrIS: S-NPP satellite
  - LMDz-OR-INCA chemistry transport model
    - calculate ammonia lifetime: $\tau = C/L$, C: concentration, L: total loss
    - simulate ammonia concentrations
- Method:
  - Inverse Distance Weighting (IDW) interpolation: oversampling methods
  - Emission flux calculation: a 1–dimensional box model
    - $E = M/\tau$, M: NH3 mass
- Results:
  - Modelled lifetime: 11.6±0.6 hours
  - Satellite-constrained emissions
  - Average
  - Seasonal variability
  - Comparison with emissions applying a constant lifetime of 0.5 days (Damme et al., 2018)
  - Site-specific emissions and seasonal variation





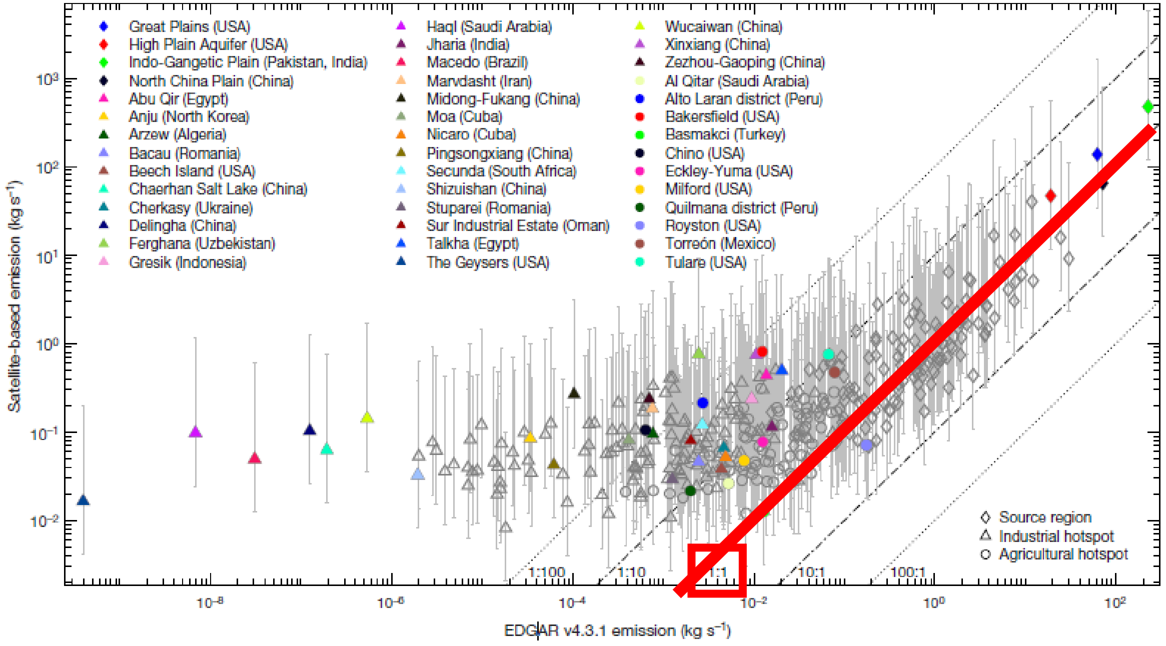


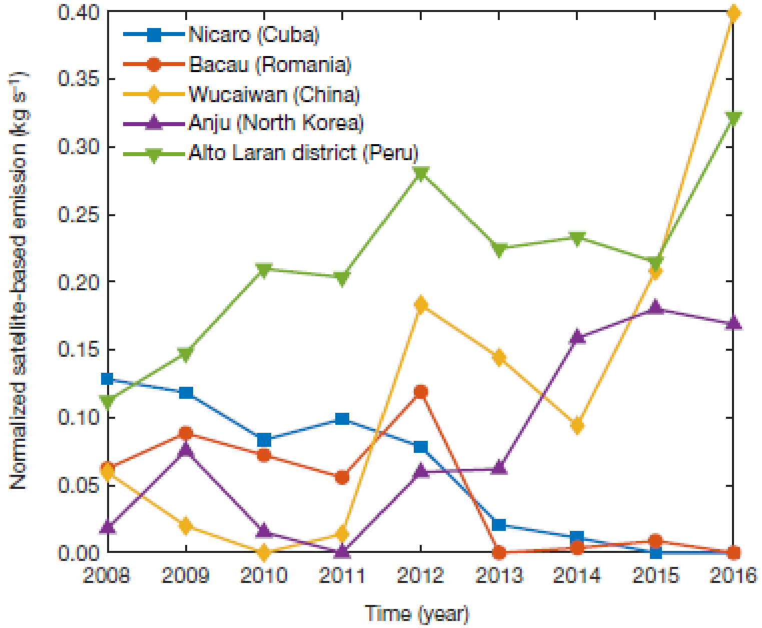


(Evangeliou et al., 2020)

Industrial and agricultural ammonia point sources exposed

- Identify, categorize and quantify the world's ammonia emission hotspots
- Observations: IASI 2008-2017
- Method:
  - Identification: manually
  - Attribution:
    - Visible imagery
    - Inventories
  - Emission flux calculations: $E = M/\tau$
- Results:
  - compared Satellite-derived emission with the inventory EDGAR
  - satellite-based ammonia emission trends

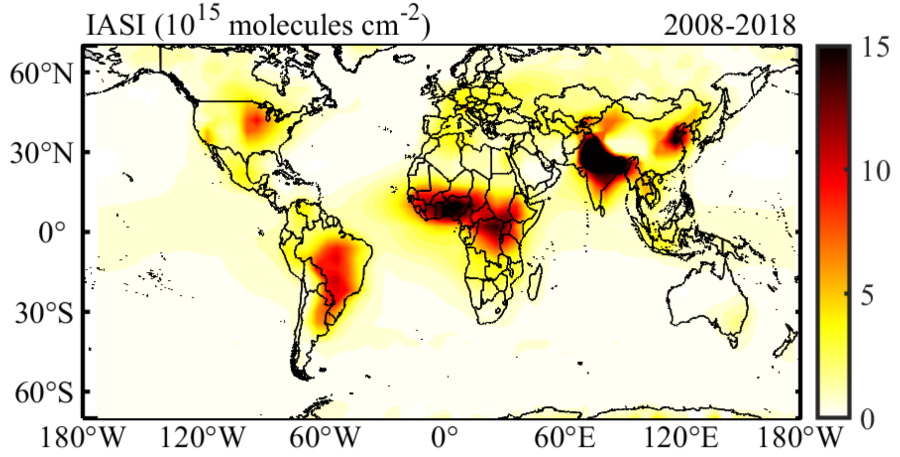


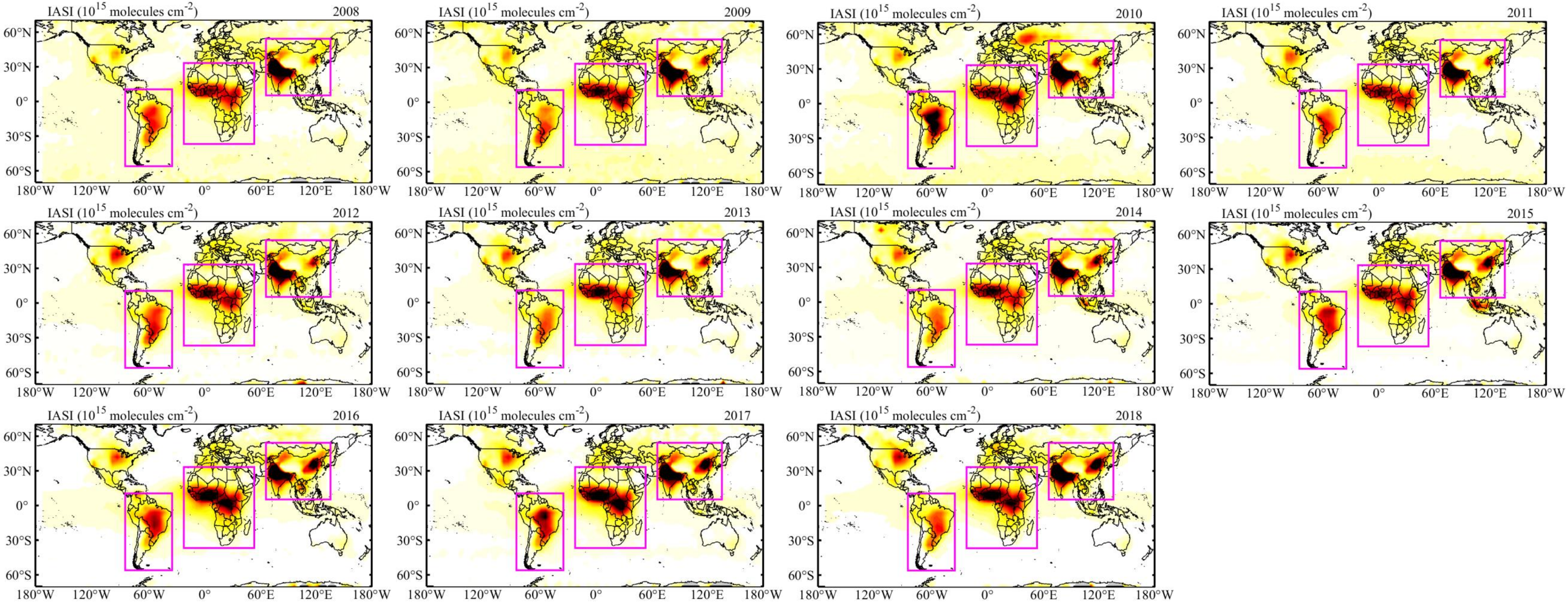


(Damme et al, 2016)

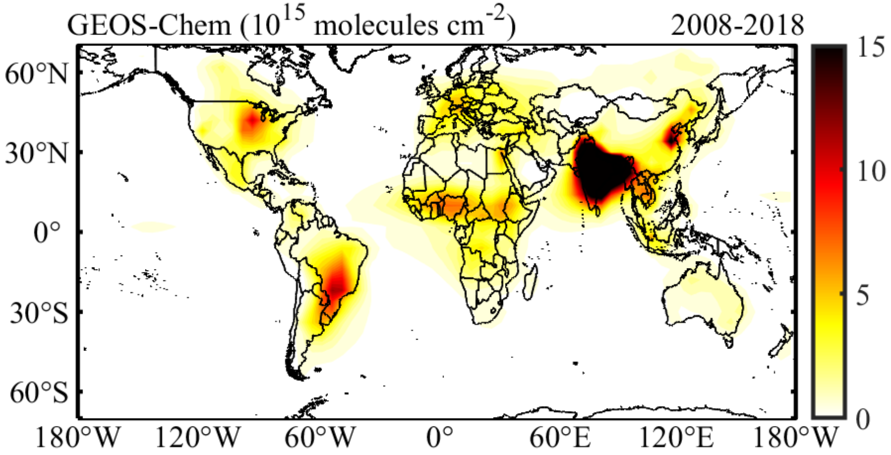
results

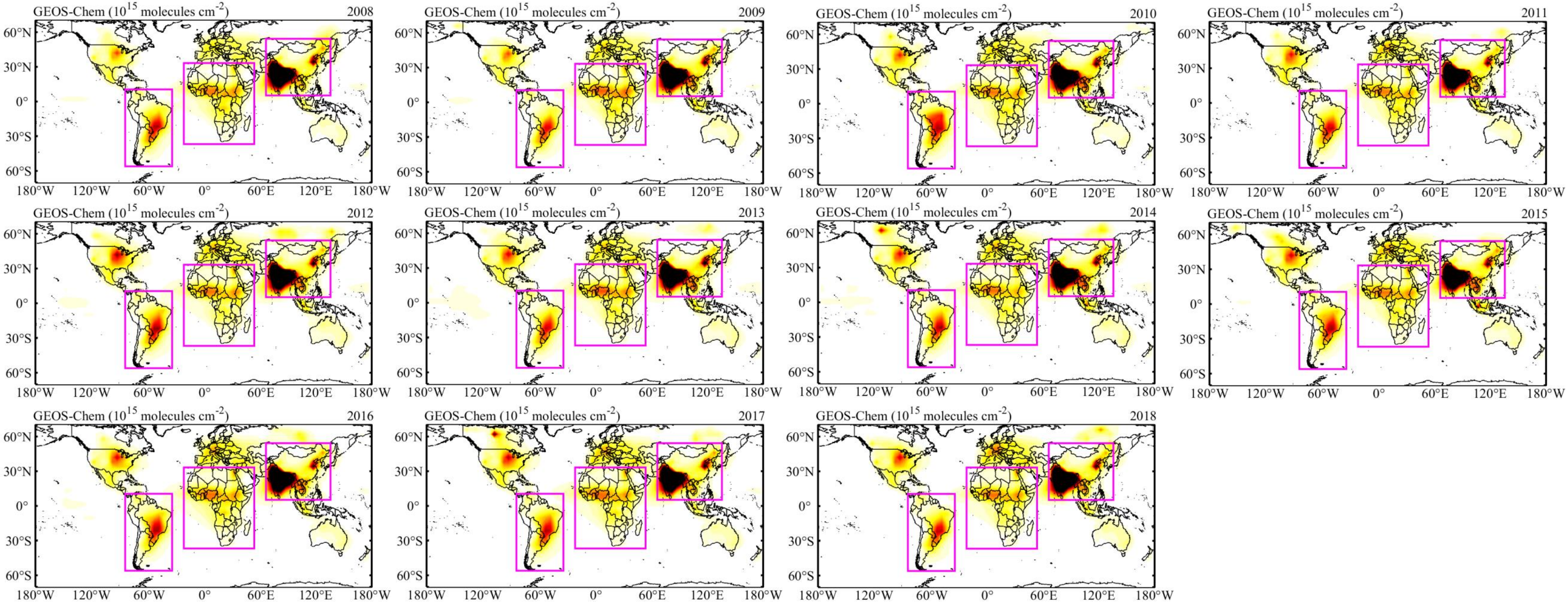
IASI mean in annual concentration distribution



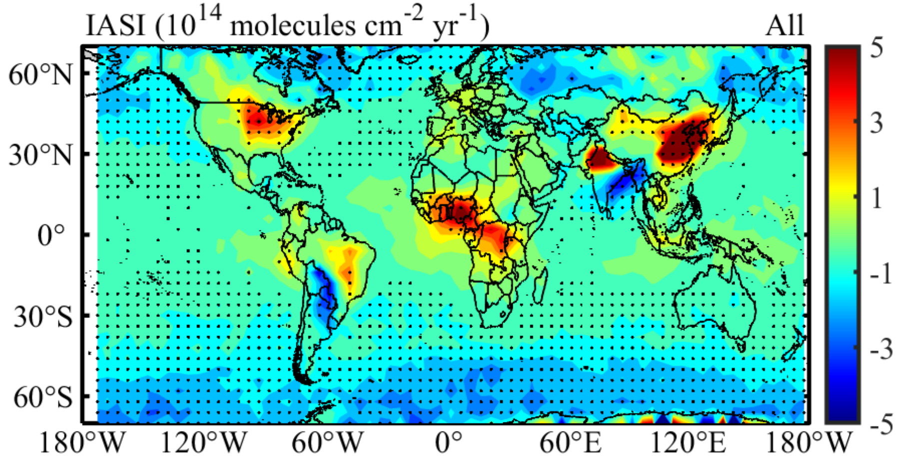


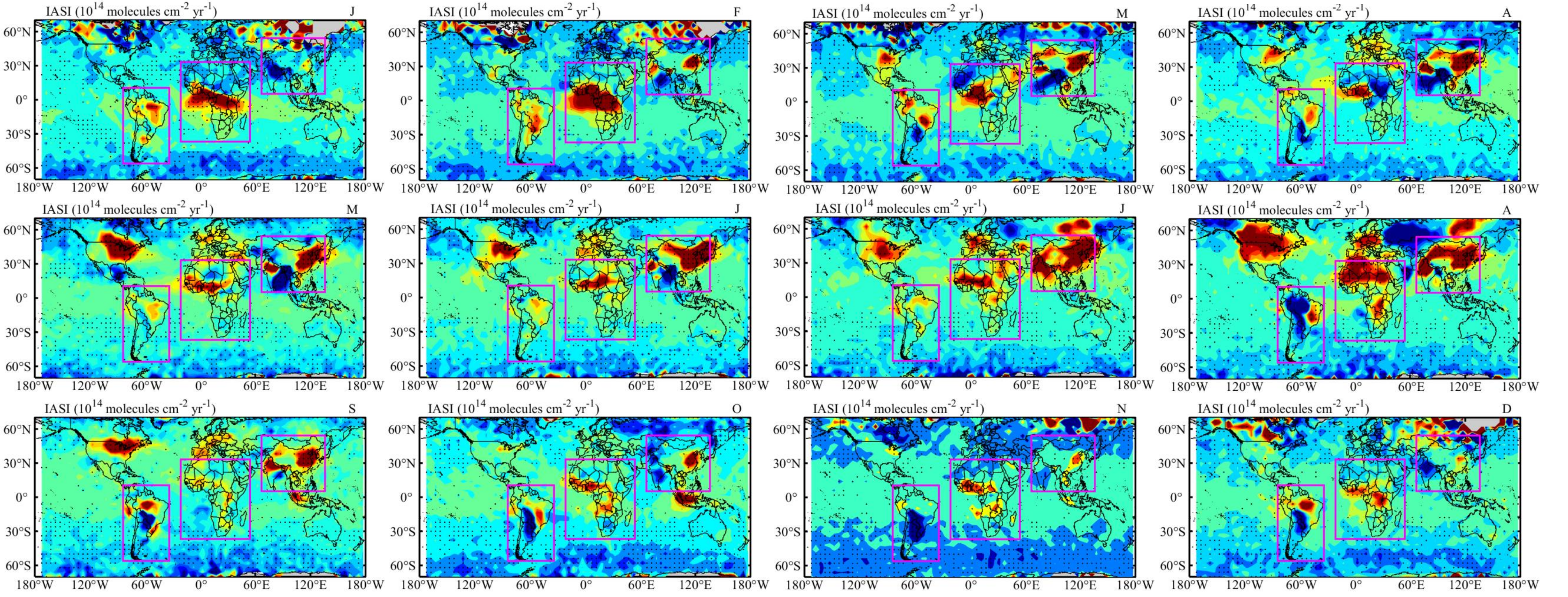
GEOS-Chem mean in annual concentration distribution



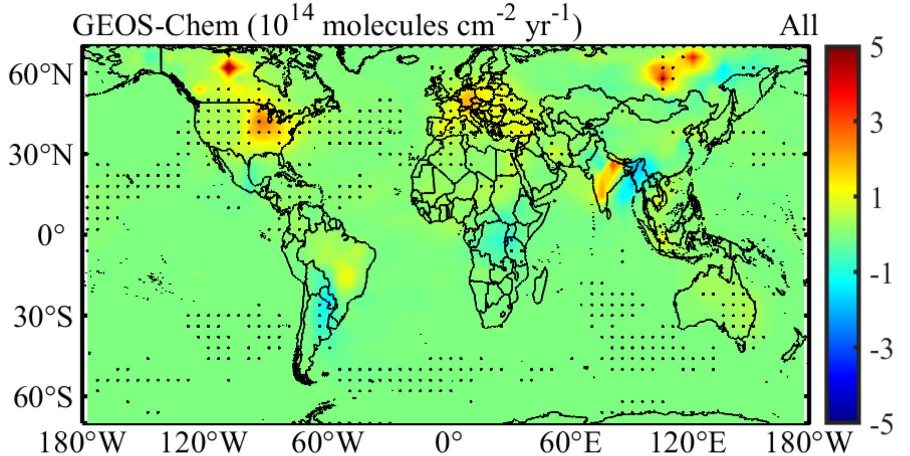


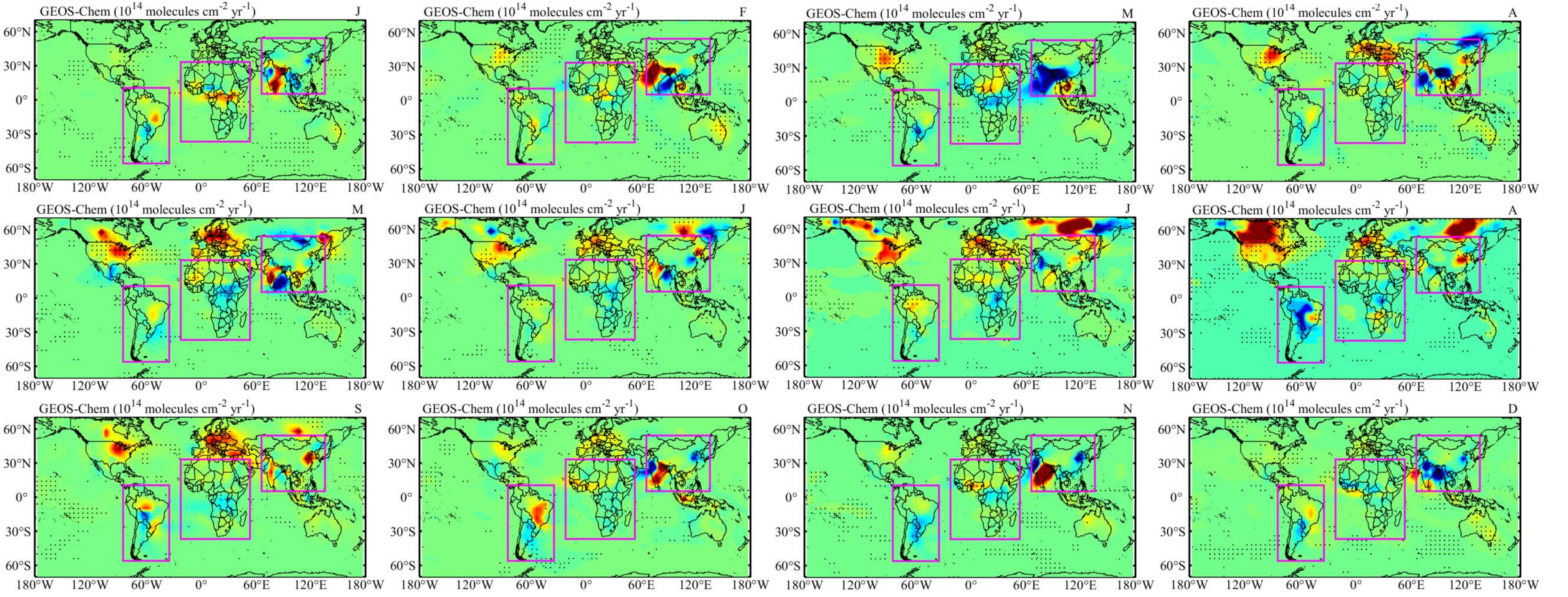
IASI trend in monthly concentration distribution





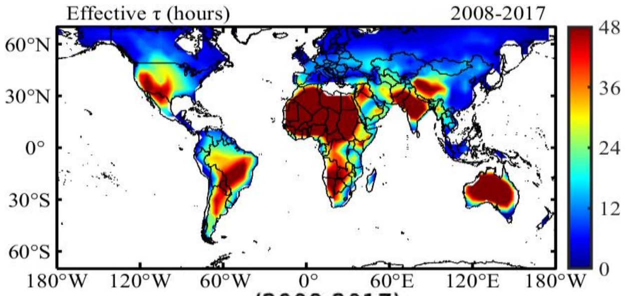
GEOS-Chem trend in monthly concentration distribution

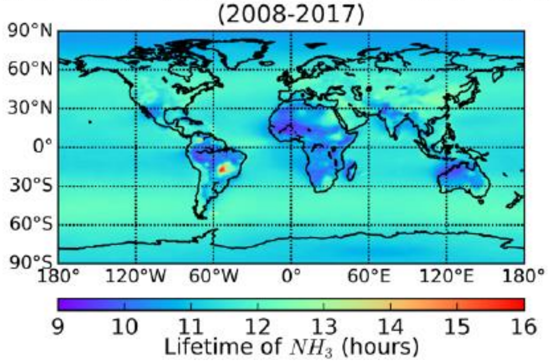


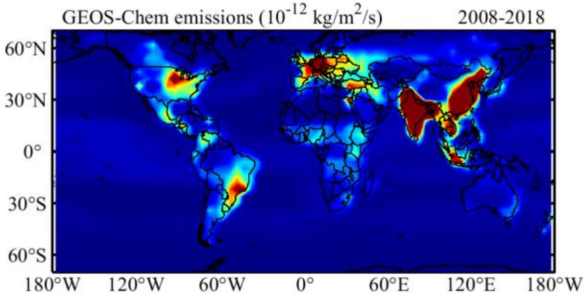


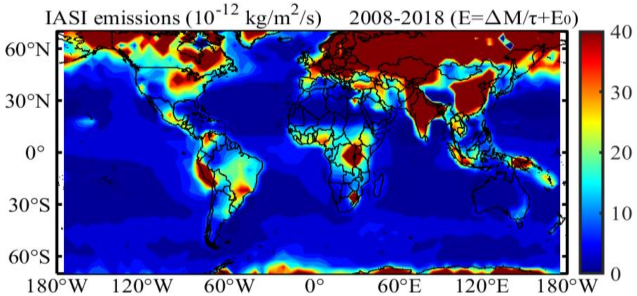
Effective lifetime and correspond emissions

- Ammonia-water equilibrium
  - $NH_3 + H_2O \rightleftharpoons NH_3 \cdot H_2O$
  - $H_{NH_3} = \frac{[NH_3 \cdot H_2O]}{\mathrm{p}_{NH_3}}$, Henry's Law
  - $NH_3 \cdot H_2O \rightleftharpoons NH_4^+ + OH^-$
  - $K_1 = \frac{[NH_4^+][OH^-]}{[NH_3 \cdot H_2O]}$
  - $[NH_4^+] = \frac{K_1 * H_{NH_3}}{[OH^-]} \mathrm{p}_{NH_3} = K_{NH_4^+/NH_3} * C_{NH_3}$
- $\tau_{mod} = \frac{M_{NH_3} + M_{NH_4^+}}{-(\nabla M_{NH_3,}^{drydep,wetdep} + \Delta M_{NH_3}^{drydep,wetdep})} = \frac{(K_{NH_4^+/NH_3}^{\mathrm{mod}} + 1) M_{mod}}{-\Delta M_{NH_3,NH_4^+}^{drydep,wetdep}}$
- Effective $\tau_{mod} = \frac{\tau_{mod}}{K_{NH_4^+/NH_3}^{\mathrm{mod}} + 1} = \frac{M_{mod}}{-\Delta M_{NH_3,NH_4^+}^{drydep,wetdep}}$
- $\hat{E}_{obs} = \frac{(M_{\mathrm{obs}} - M_{mod})}{\tau_{mod}} + E_{mod}$



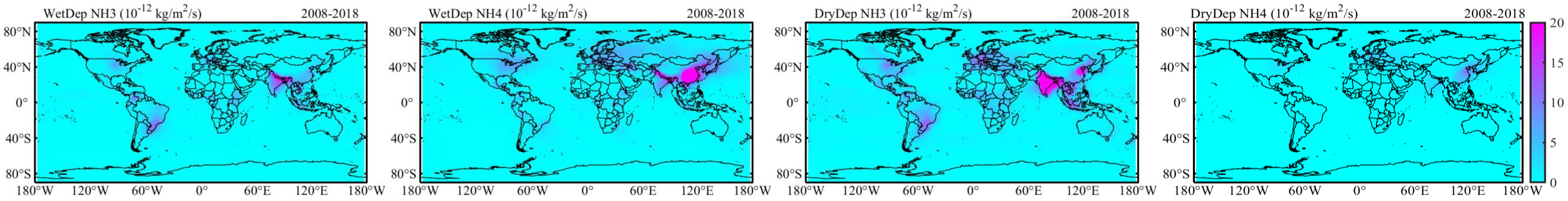


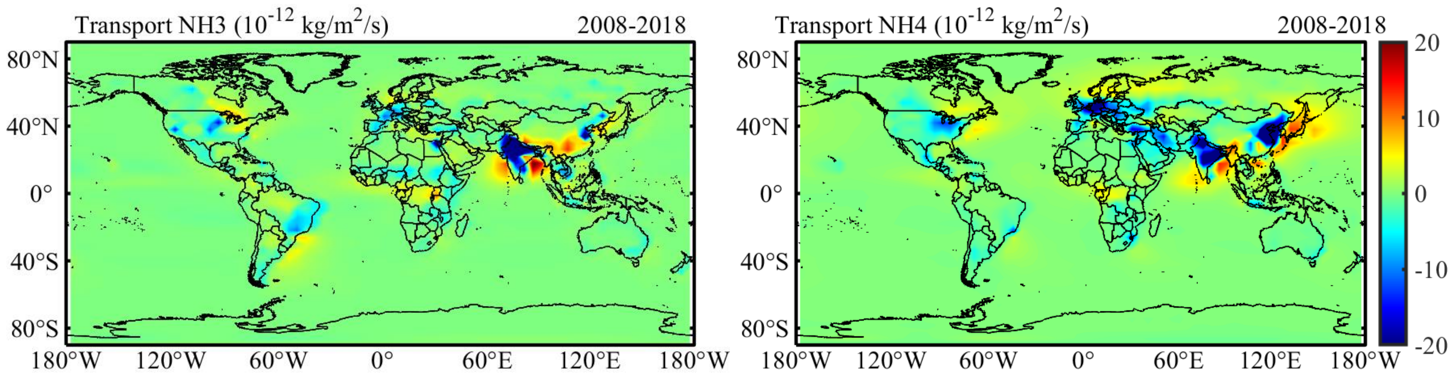




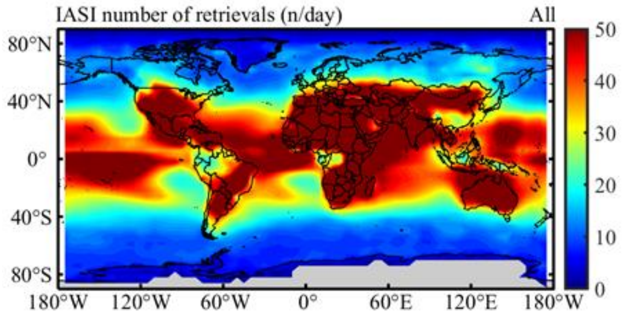
(Evangeliou et al., 2020)

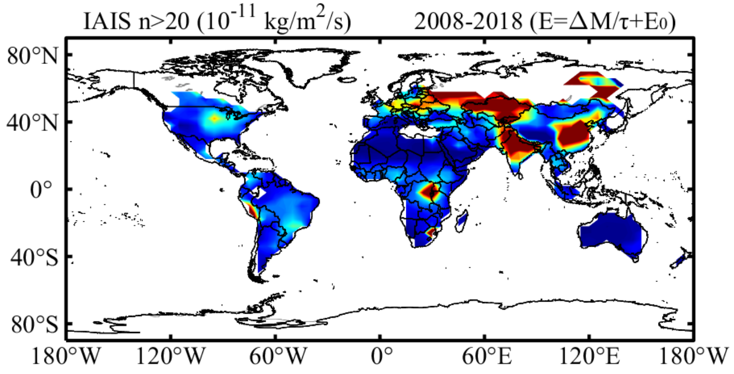
GEOS-Chem deposition and transport

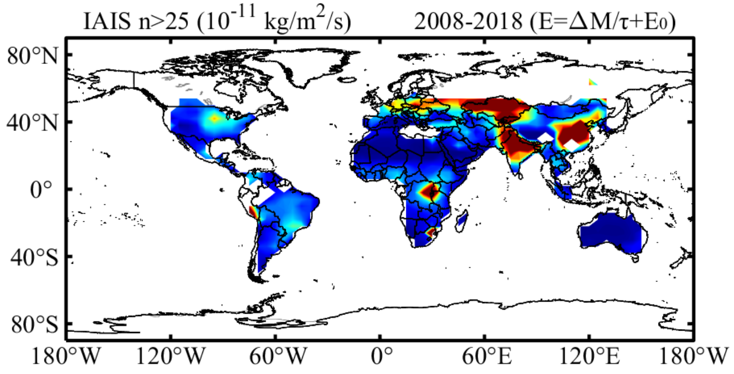


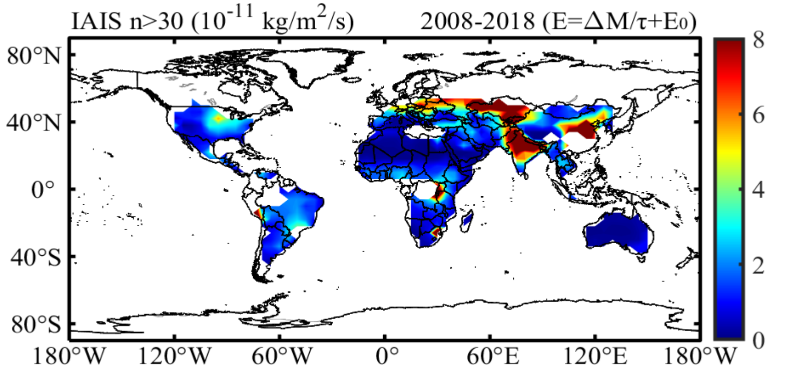


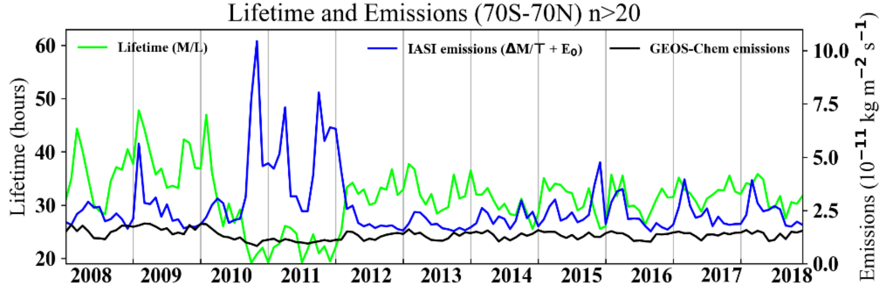
IASI emission filtered again by the number of retrievals in a grid

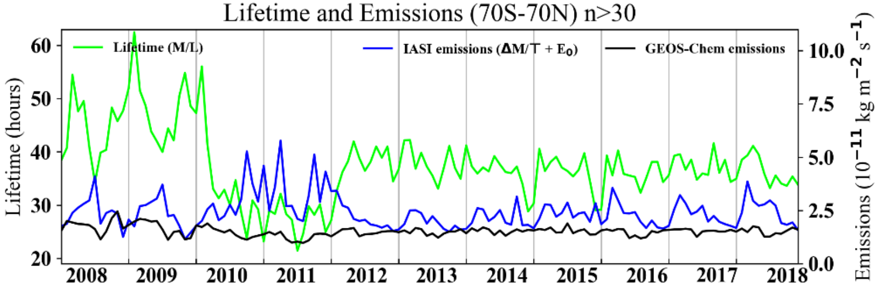


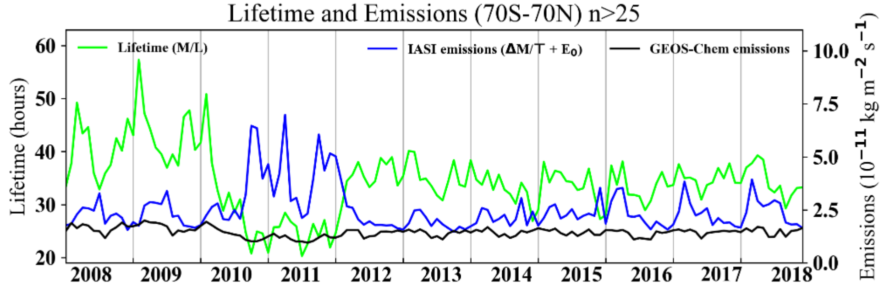


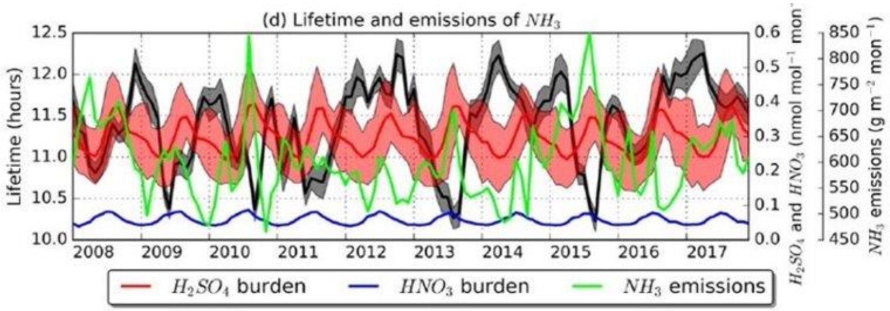












(Evangeliou et al., 2020)

GEOS-Chem total column concentration

- $\Omega = \sum_{i=1}^{47} c_{\mathrm{i}} \times rho_i \times h_i$
  - Ω**: total column concentration,** [mol/m2]
  - c_{i}: 'IJ-AVG-$_NH3', mixing ratio for each level, [ppbv] to [v/v] (*1E-9)
  - rho_i: 'TIME-SER_AIRDEN', air density for each level, [molecules/cm3]
  - h_i: 'BXHGHT-$_BXHEIGHT', grid box height for each level, [m] to [cm] (*100)

Regrid 180x360 to 46x72

- Latitude: 46 degrees
  - 88°-90°: 2x5 to 1x1, 2 degrees
  - 0-88°: 4x5 to 1x1, 44 degrees
- Method:
  - Step1: mask ocean, set as NaN
  - Step2: calculate mean value in each upscaling grid

emissions

- Anthropogenic
  - APEI: Historical Canadian emissions (1990-2014)
  - NEI2011_MONMEAN: US emissions
  - MIX: Asian anthropogenic emissions
  - DICE_Africa: emissions from inefficient combustion over Africa
  - CEDS: Global anthropogenic emissions
  - POET_EOH: aldehydes and alcohols
  - TZOMPASOSA: global fossil fuel and biofuel emissions of C2H6 for 2010
  - XIAO_C3H8: C2H6 and C3H8
  - AFCID: PM2.5 dust emission
- Natural
  - GEIA_NH3: 1990 (obsolete now)
  - SEABIRD_DECAYING_PLANTS: the oceanic emissions of acetaldehyde
  - NH3: the Arctic seabird
- Biomass burning
  - GFED4: biomass burning emissions
- Ship
  - CEDS_SHIP
  - SHIP

End