Ammonia observation and modeling simulation 5

IASI data and GEOS-Chem simulation

2020.11

- Accomplished:
  - 1. seasonal mean distribution of GEOS-Chem over 2008-2018
  - 2. seasonal trend distribution of GEOS-Chem over 2008-2018
  - 3. literature: NH3 Retrievals of IASI
  - 4. literature: NH3 emission from IASI and GEOS-Chem over the U.S.
  - 5. literature: validate IASI NH3 by ground-based Fourier transform infrared spectroscopy measurements (FTIR)
- Ammonia Data:
  - IASI total columns, 1°×1°, monthly
    - Reanalyzed IASI/Metop-A (2008-2018) L3
  - GEOS-Chem simulation, 4°×5°, daily
    - column concentration (2008-2018)
- Ongoing:
  - 1. consider the cause of trend
  - 2. comparison of IASI observation and GEOS-Chem simulation

Version 2 of the IASI NH3 neural network retrieval algorithm: reanalysed datasets

- several improvements to the original neural-network-based retrieval
- how to post-process, treat and interpret the data
- introduce ANNI-NH3-v2.1R-I,

Version 2 of the IASI NH_3 neural network retrieval algorithm: near-real-time and reanalysed datasets

Martin Van Damme[1], Simon Whitburn[1], Lieven Clarisse[1], Cathy Clerbaux[1,2], Daniel Hurtmans[1], and Pierre-François Coheur[1]

[1]Université libre de Bruxelles (ULB), Atmospheric Spectroscopy, Service de Chimie Quantique et Photophysique, Brussels, Belgium
[2]LATMOS/IPSL, UPMC Univ. Paris 06 Sorbonne Universités, UVSQ, CNRS, Paris, France

Correspondence: Martin Van Damme (martin.van.damme@ulb.ac.be)

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

- an improved retrieval scheme for near real-time global NH3 retrievals from IASI
  - the main characteristics of IASI
  - the retrieval method
  - the global distributions of NH3
  - the trends in NH3 concentrations over five years of IASI operation

Retrievals of atmospheric ammonia (NH3) from IASI satellite observations

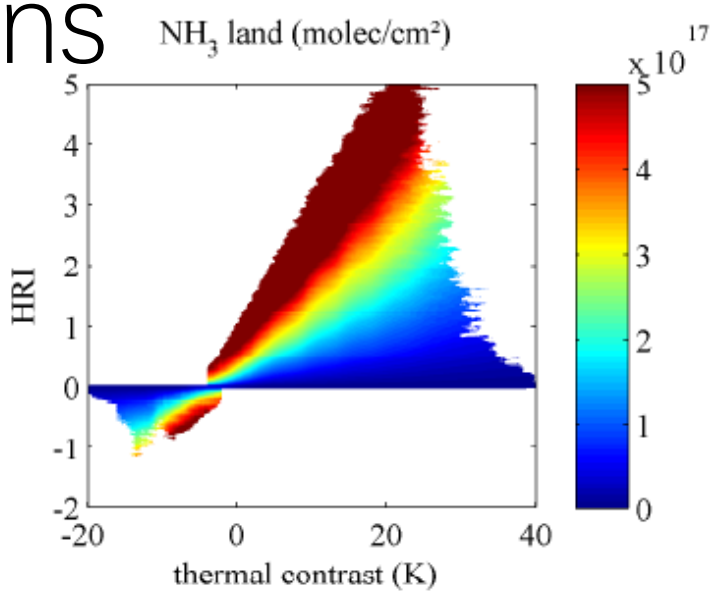
- IASI: identify 24 atmospheric species
- NH3 Retrievals
  - retrieval schemes:
    - relies on the detection algorithm of Walker et al. (2011)
    - the brightness temperature differences to column conversion from Clarisse et al. (2009)
  - hyperspectral range index (HRI): providing in a single retrieval step a quantity that is representative of the NH3 abundance, without having to retrieve other parameters
    - y: a measured spectrum
    - $\overline{y}$: a mean background spectrum
    - G:the measurement contribution function
    - S: variance-covariance matrix
    - K: the difference between a spectrum simulated with a given amount and a spectrum simulated without NH3

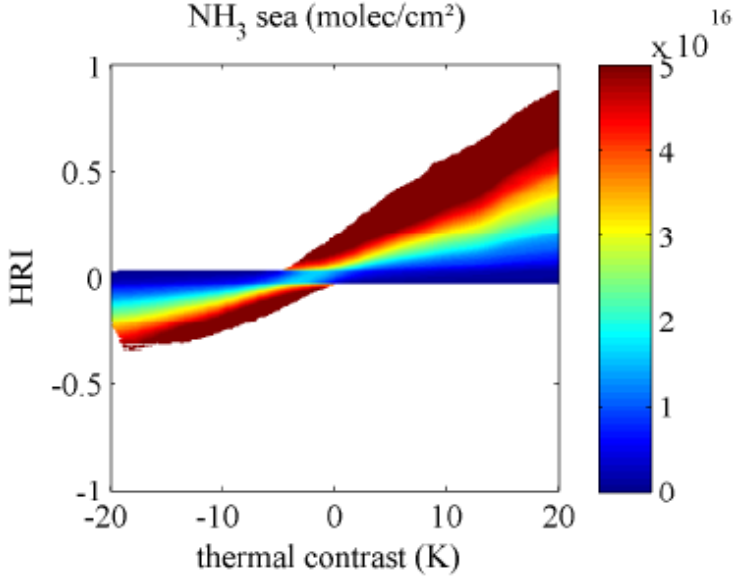
$$\mathrm{HRI} = \mathbf{G}(\mathbf{y} - \overline{\mathbf{y}})$$

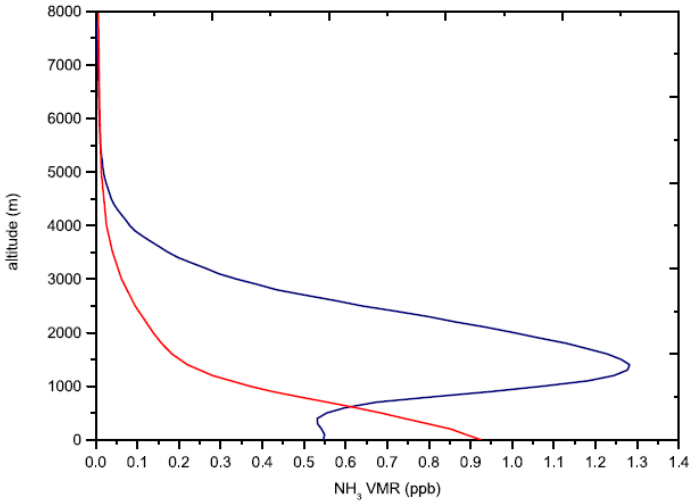
$$\mathbf{G} = (\mathbf{K}^T \mathbf{S}_y^{\mathrm{obs}\,-1} \mathbf{K})^{-1} \mathbf{K}^T \mathbf{S}_y^{\mathrm{obs}\,-1}.$$

Retrievals of atmospheric ammonia (NH3) from IASI satellite observations

- IASI: identify 24 atmospheric species
- NH3 Retrievals
  - look-up tables (LUTs): link the HRI to the NH3 column concentration and thermal contrast
    - Use NH3 GEOS-Chem model profiles above land and sea
    - built from about 450 000 simulated IASI spectra above land and about 116 000 above sea







(Damme et al, 2014)

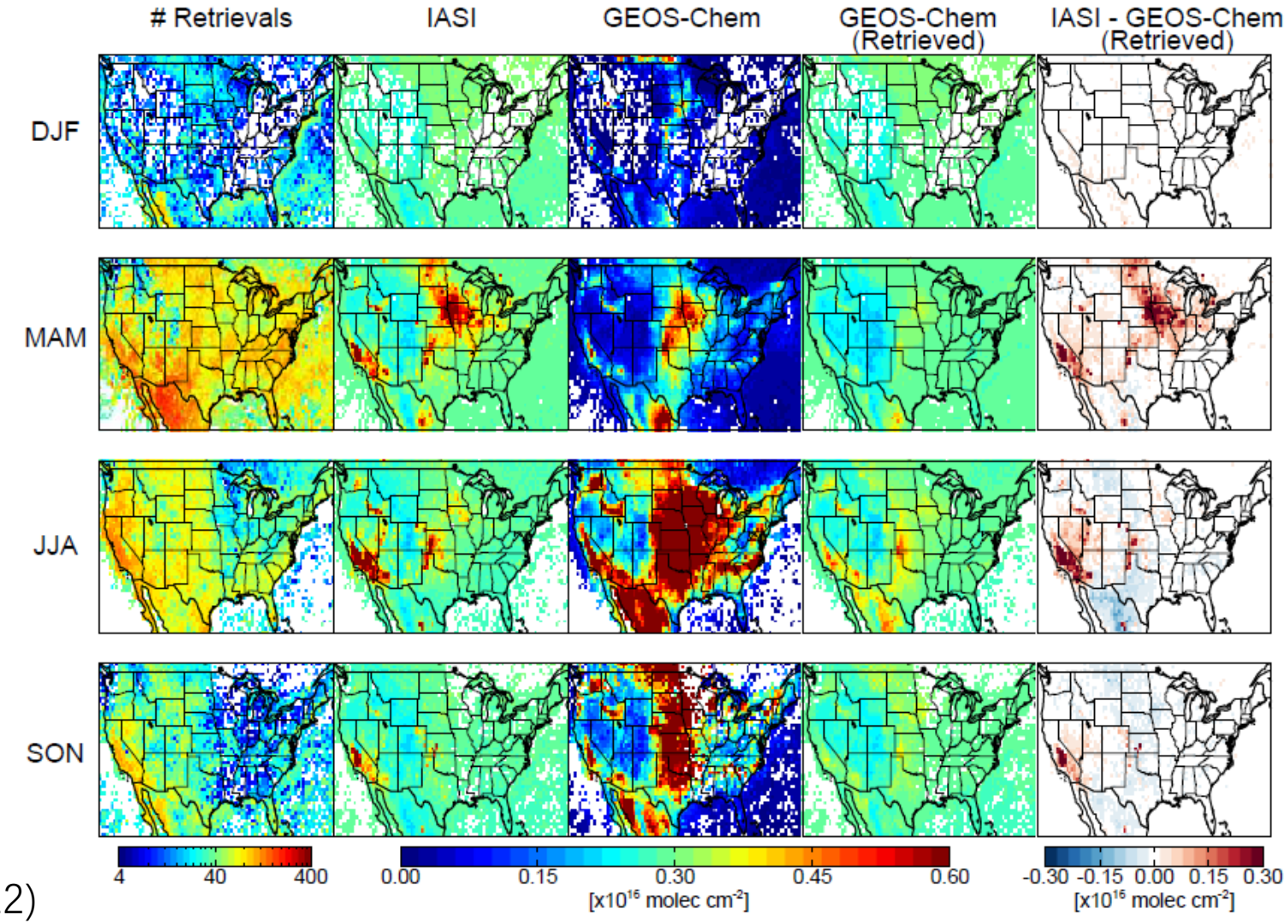
Atmospheric ammonia and particulate inorganic nitrogen over the United States

- investigate the skill of the GEOS-Chem global model in reproducing regional ammonia loadings and inorganic concentrations and partitioning
- IASI Ammonia retrievals: formal optimal estimation methods (Rodgers, 2000)
  - profile of ammonia
  - x: true profile
  - x_a: a constant global moderately polluted mean profile from the TM5 model
  - ε: the spectral measurement error
  - A: averaging kernel, describe the vertical sensitivity of the instrument and depend on the thermal contrast and vertical distribution of ammonia

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \varepsilon$$

Atmospheric ammonia and particulate inorganic nitrogen over the United States

- Investigating ammonia emissions
  - atmospheric ammonia column concentrations observed by IASI and simulated with the baseline GEOS-Chem model
    - cloud coverage: fall and winter
    - high degree of reliance on the a priori in the retrieval



(Heald et al, 2012)

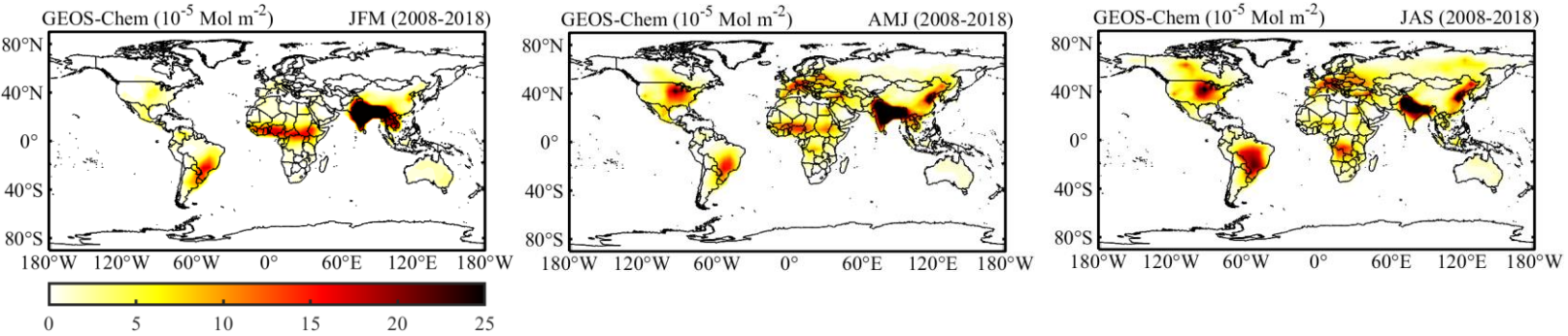
An evaluation of IASI-NH3 with ground-based Fourier transform infrared spectroscopy measurements

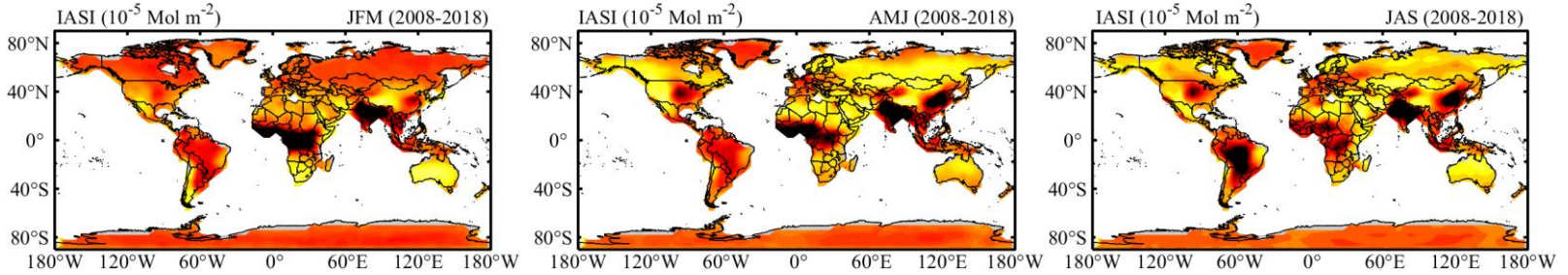
- explore the use of NH3 total columns obtained with ground-based FTIR at nine stations with a range of NH3 pollution levels to validate the IASI-NH3 satellite product by Van Damme et al. (2014a).
  - IASI-NH3 product limitations:
    - the use of only two NH3 vertical profiles:
      - a “source profile” for land cases
      - a “transported profile” for sea cases
    - not allow the calculation of an averaging kernel to account for the vertical sensitivity of the instrument sounding to different layers in the atmosphere
  - FTIR and satellite comparison methodology: Application of averaging kernels——smoothed IASI profile

$$\hat{x}_{\mathrm{sat}} = x_{\mathrm{ftir}}^{\mathrm{apriori}} + \mathbf{A}\left(x_{\mathrm{sat}}^{\mathrm{mapped}} - x_{\mathrm{ftir}}^{\mathrm{apriori}}\right)$$

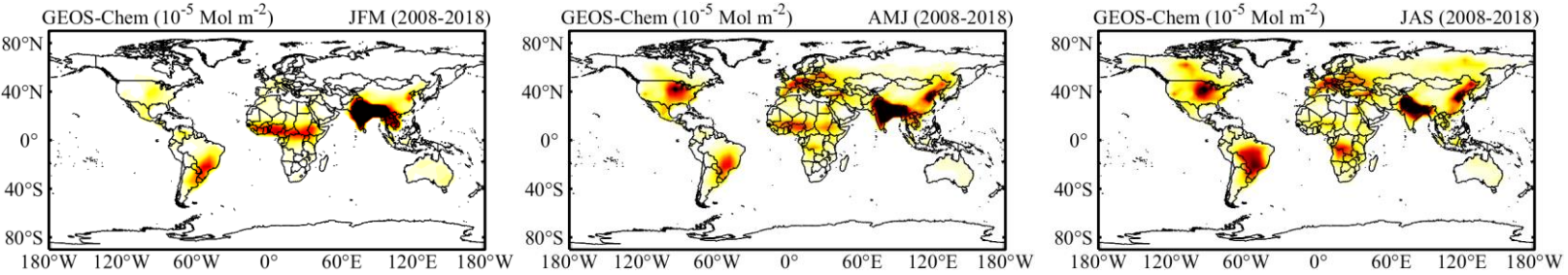
    - A: the FTIR averaging kernel
    - x_{sat}^{mapped}: The IASI profile is mapped to the altitude grid of the FTIR profile

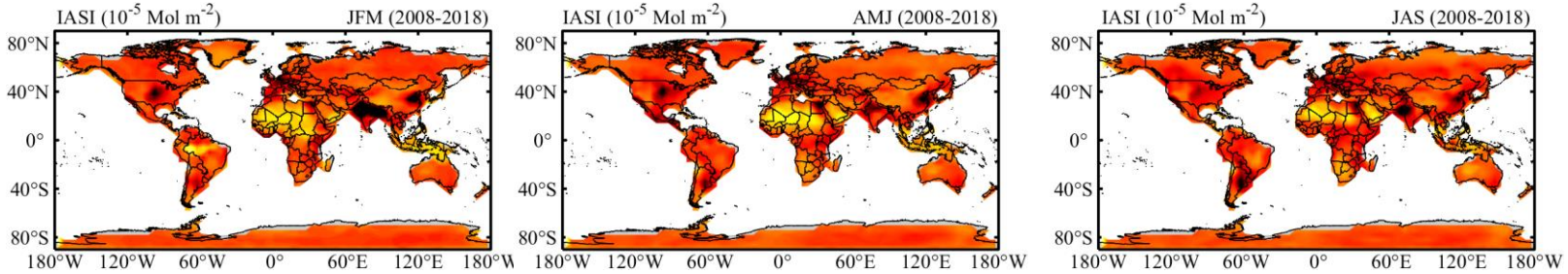
seasonal mean spatial distribution





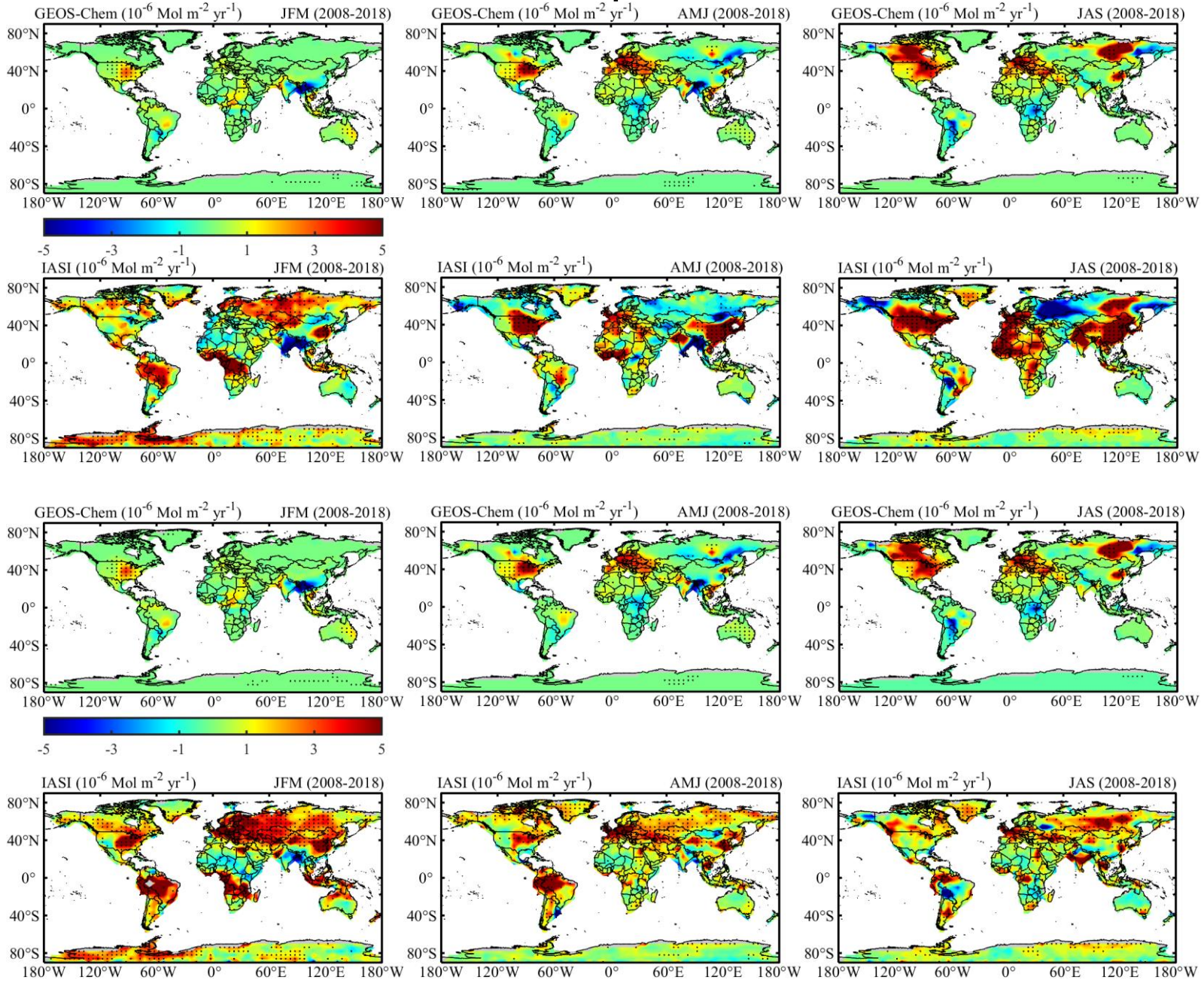
Day time





Night time

seasonal trend spatial distribution

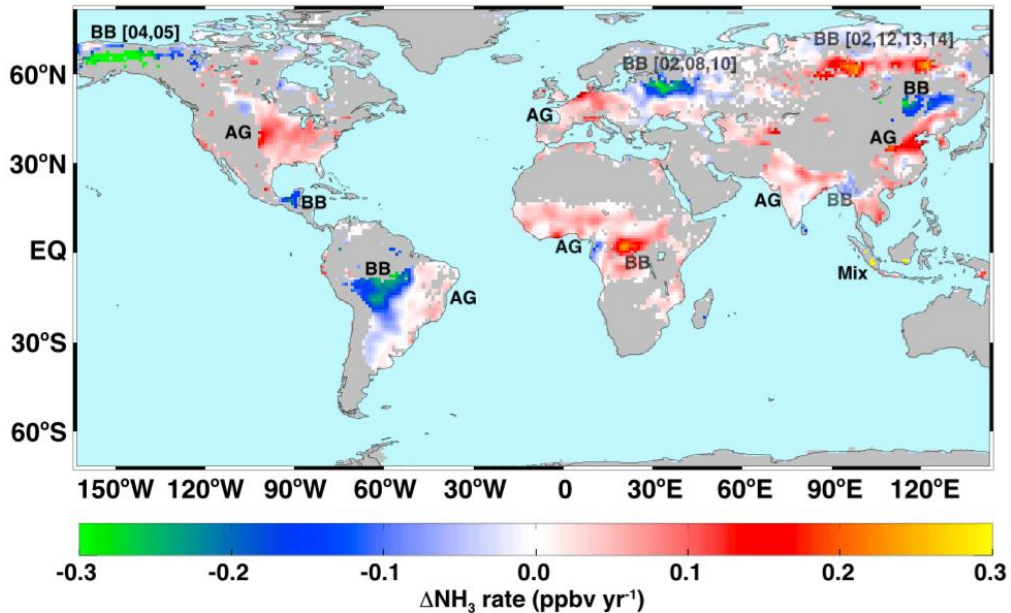


Day time

Night time

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)

total column concentration

- $\Omega = \sum_{i=1}^{47} c_{\mathrm{i}} \times rho_i \times h_i \times k$
  - 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)
  - k: 1/6.02214179E19, multiplication factor to convert [molecules/cm2] to [mol/m2]

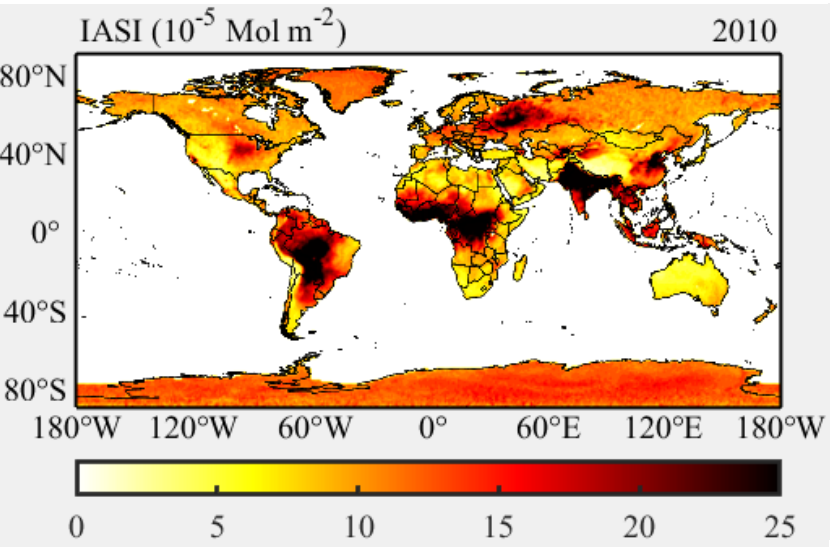
Regrid 180x360 to 46x72

- 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

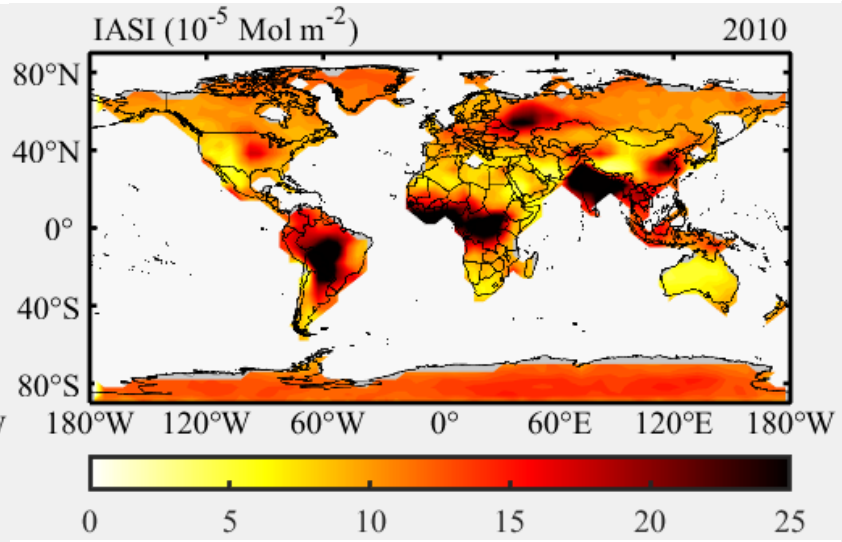
Ammonia spatial distribution

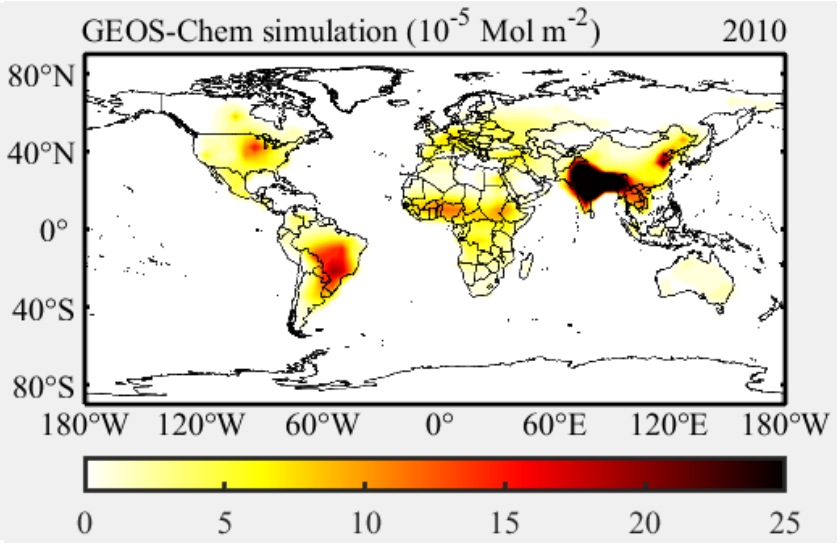
Day time

1°×1°

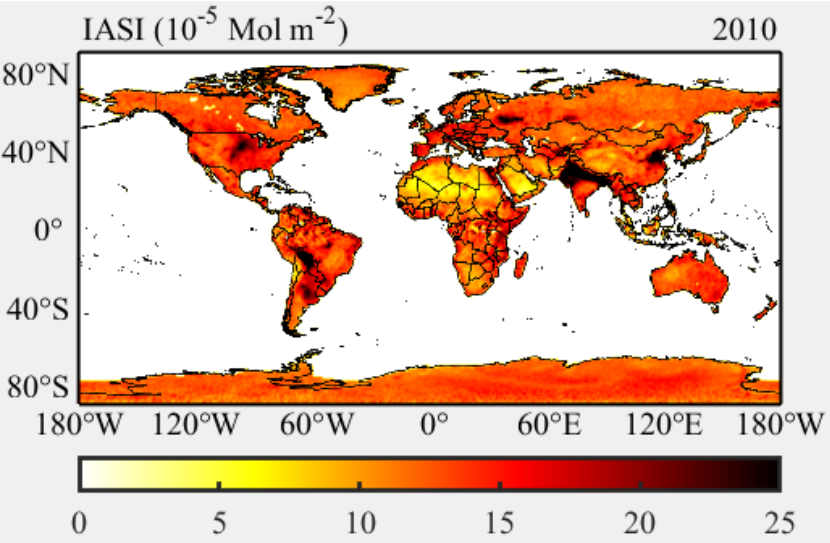


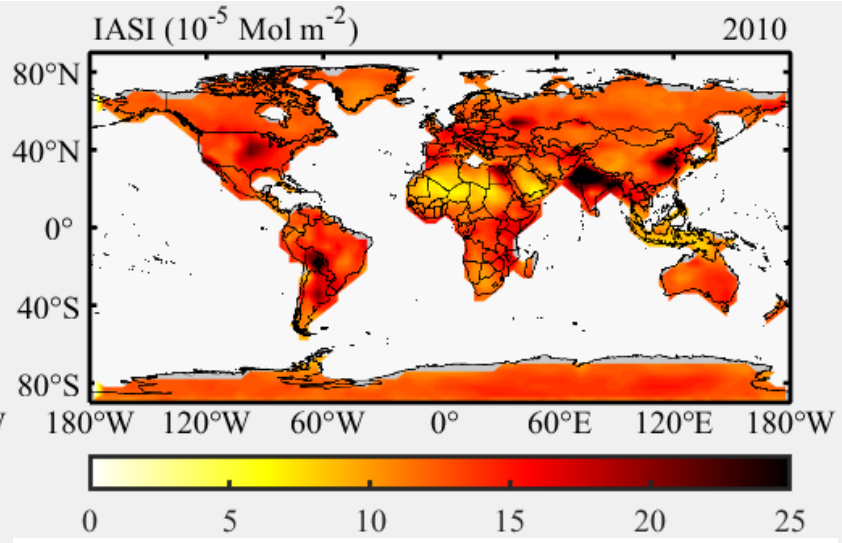
4°×5°

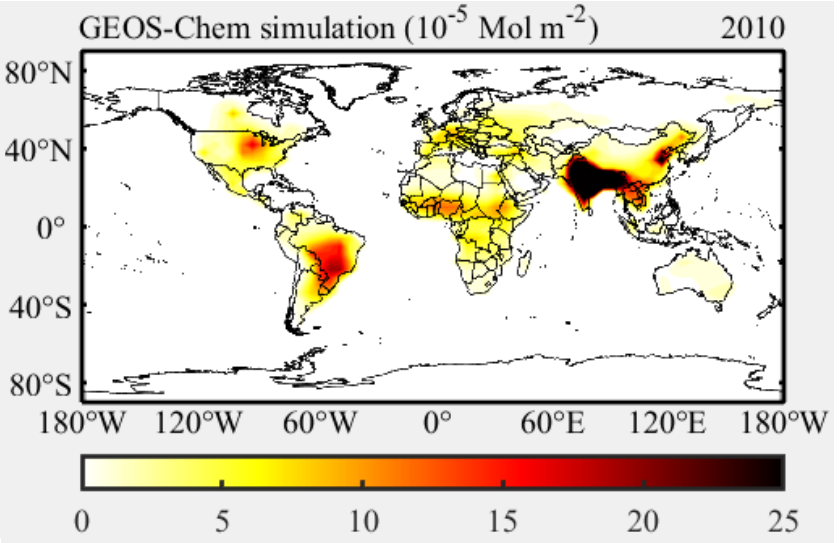




Night time

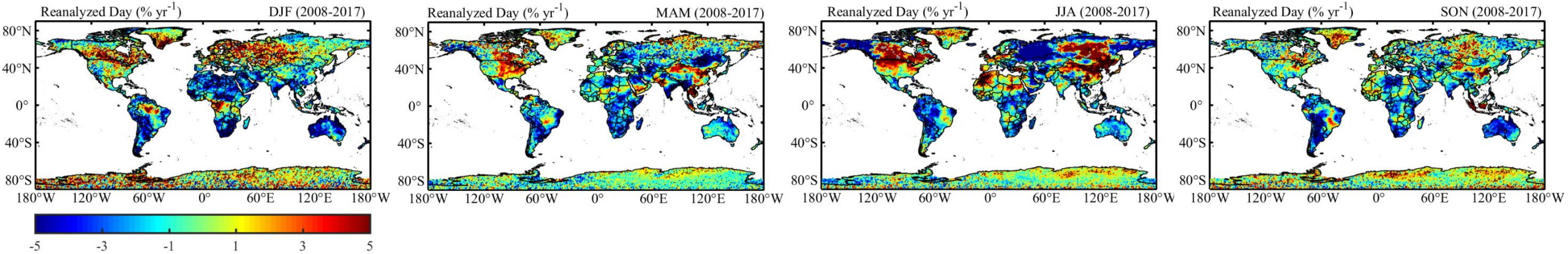




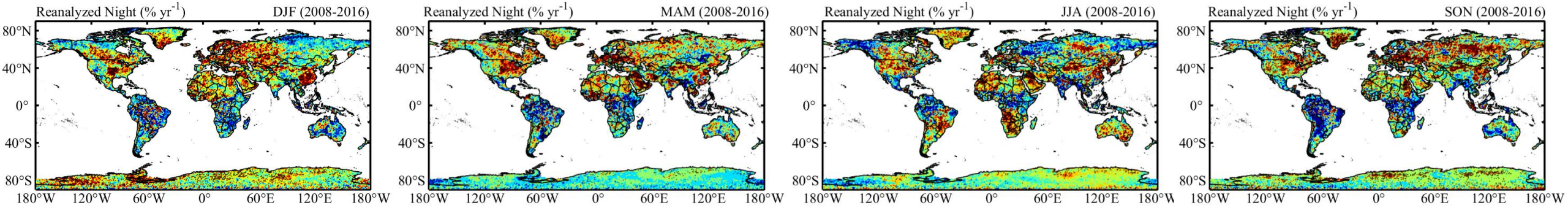


Spatial distribution of ammonia observations trend/mean

(a) day

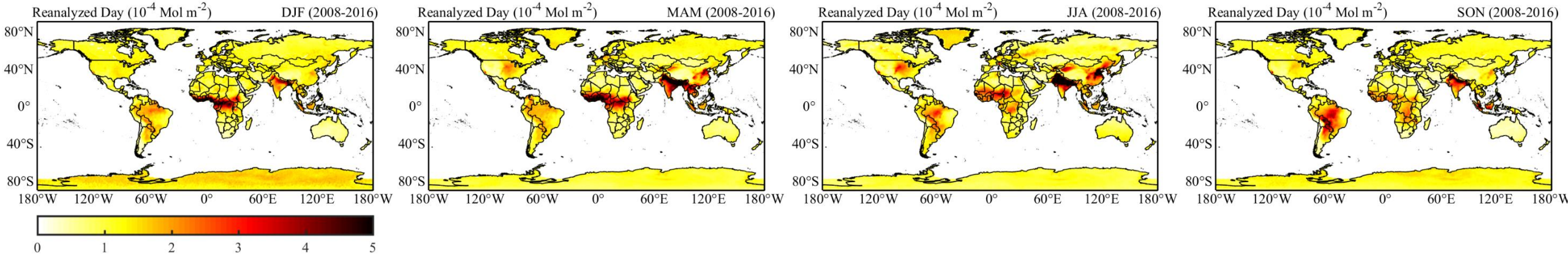


(b) night

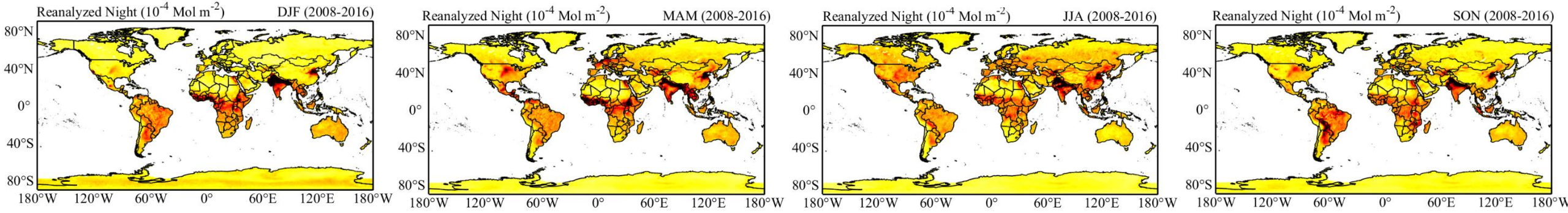


Spatial distribution of ammonia observations mean

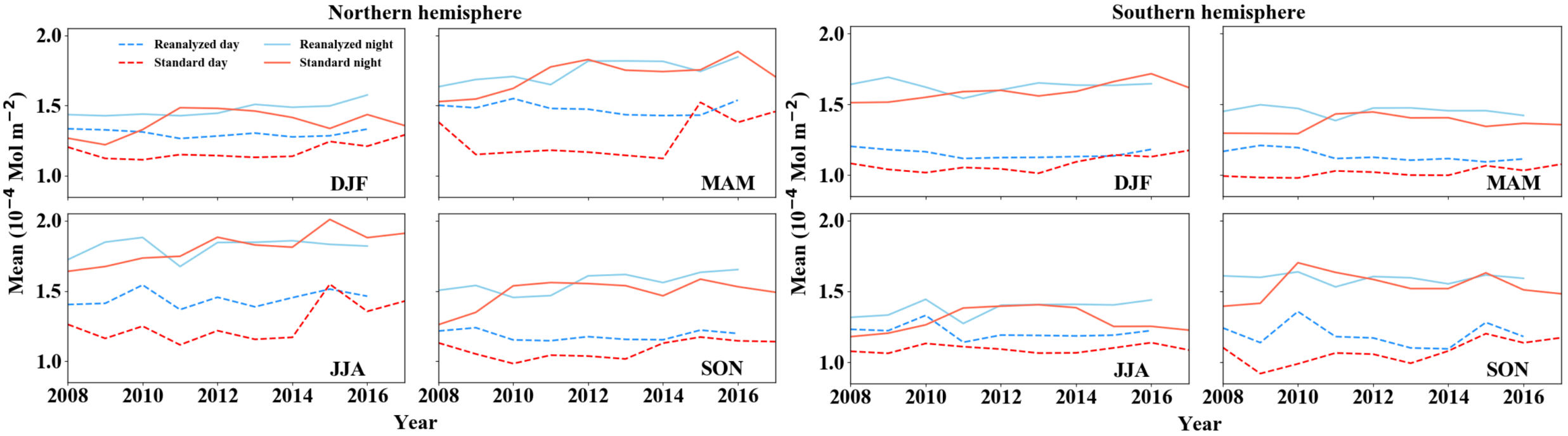
(a) day



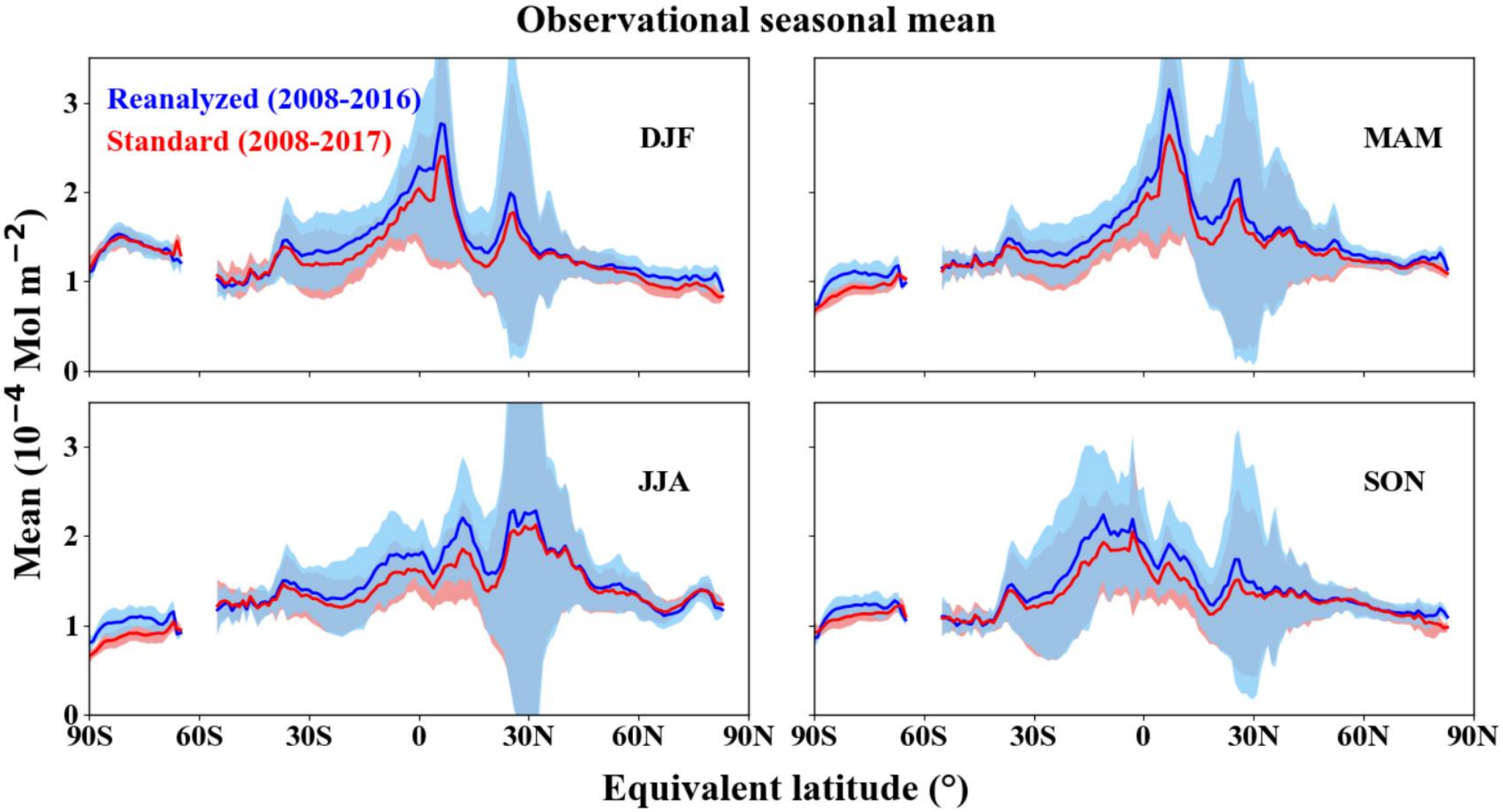
(b) night



Seasonal change for NH and SH (day and night)

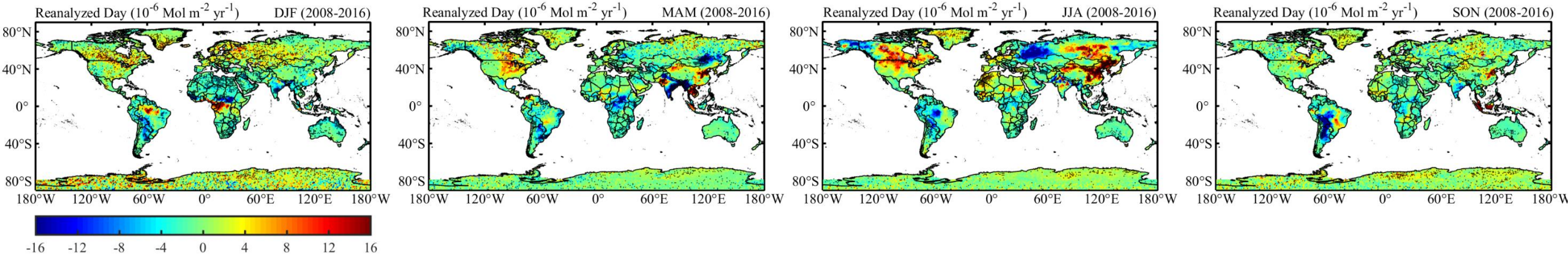


Seasonal mean of Land for equivalent latitude (within 1 sigma standard deviations)

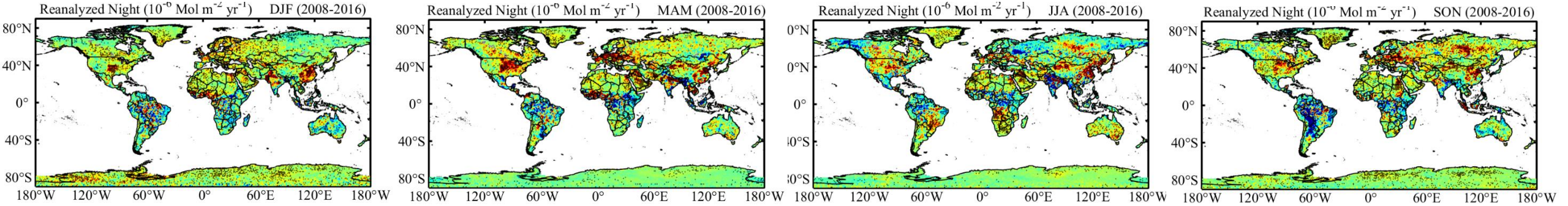


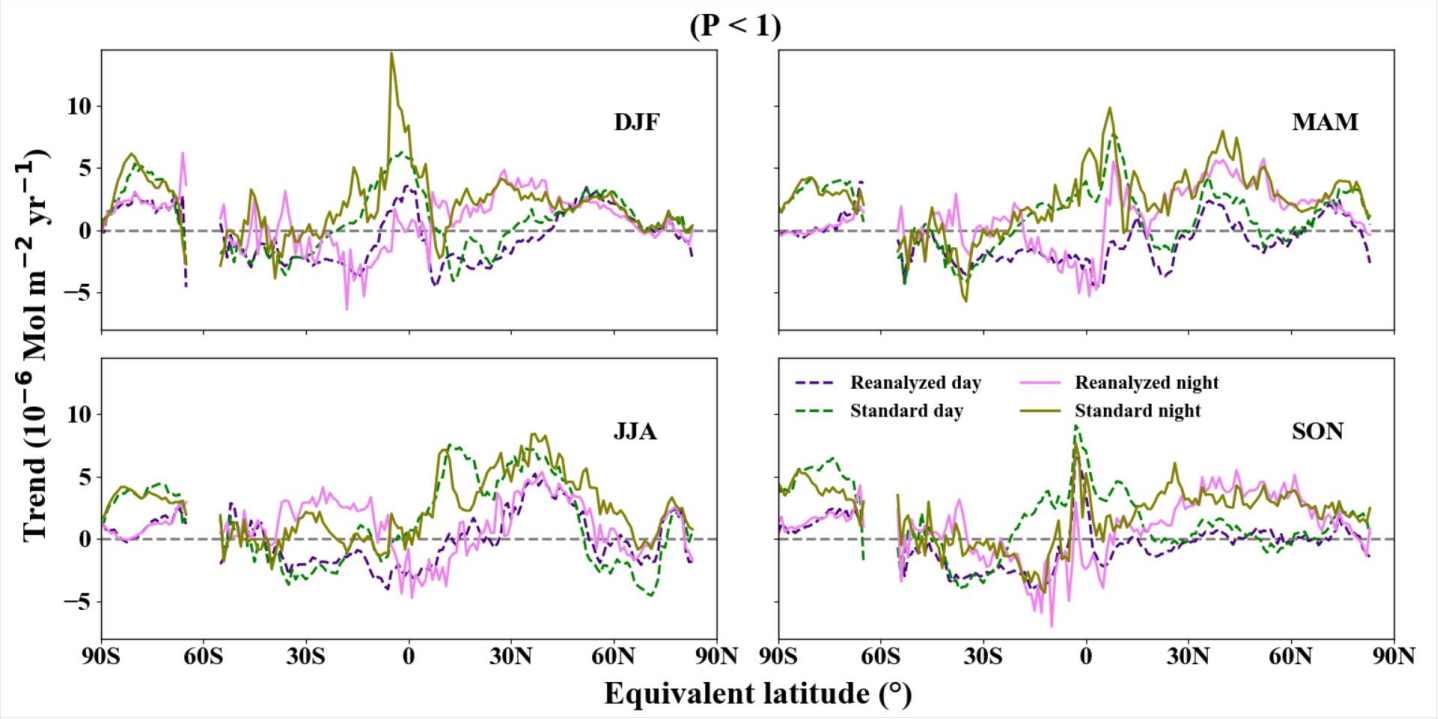
Spatial distribution of ammonia observations trend

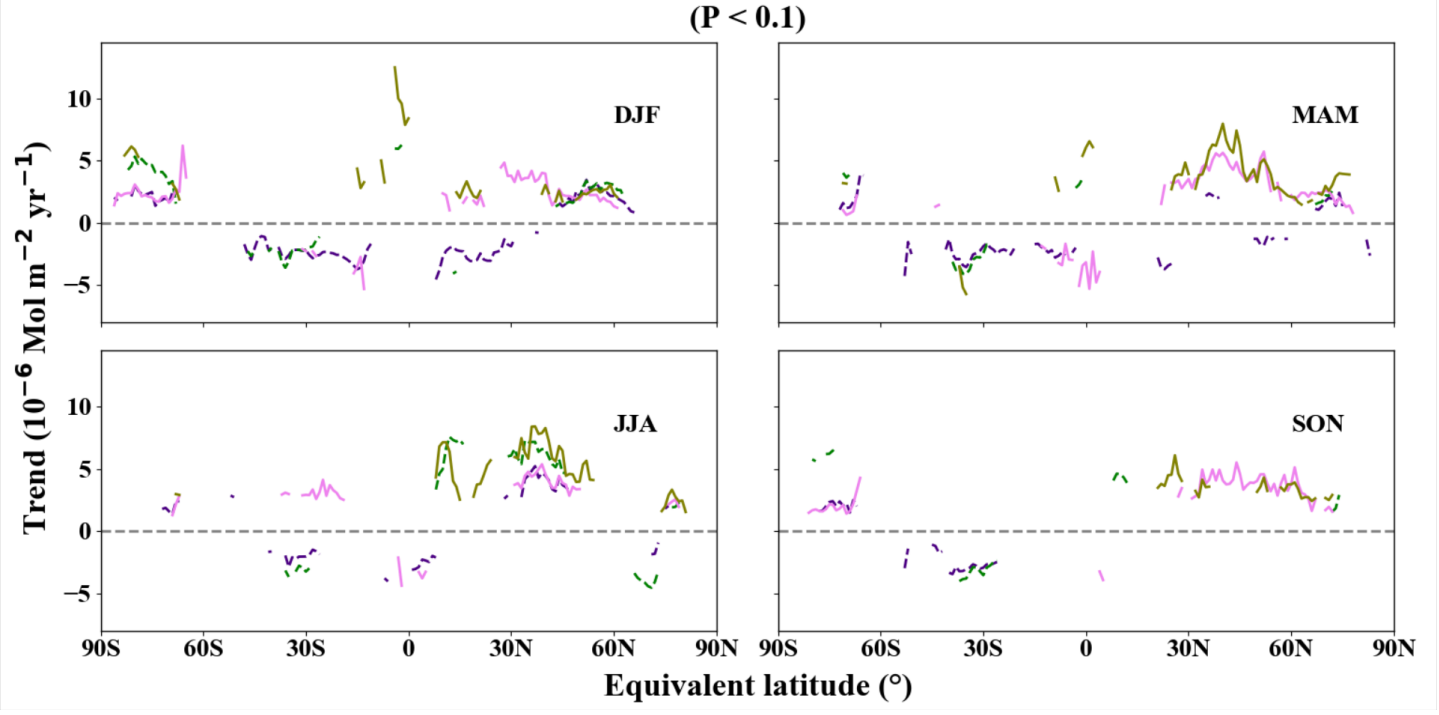
(a) day



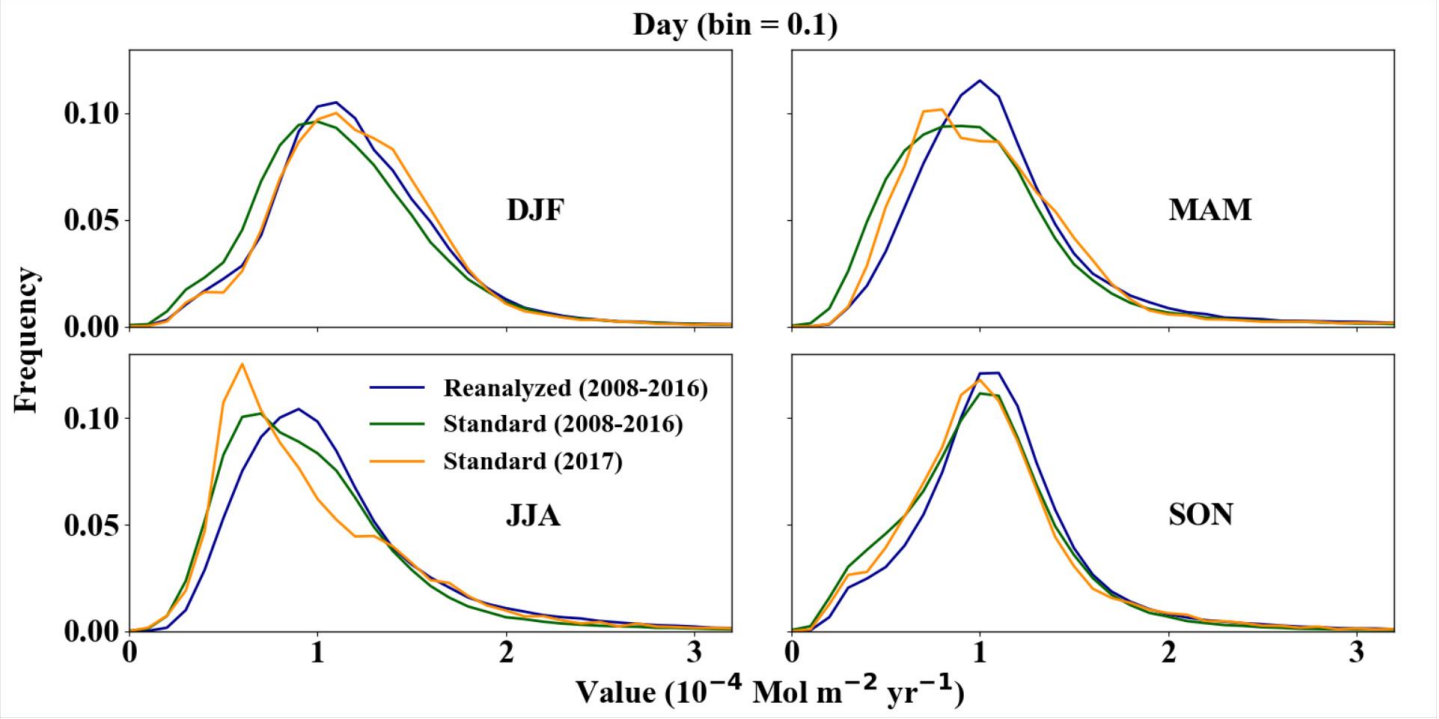
(b) night

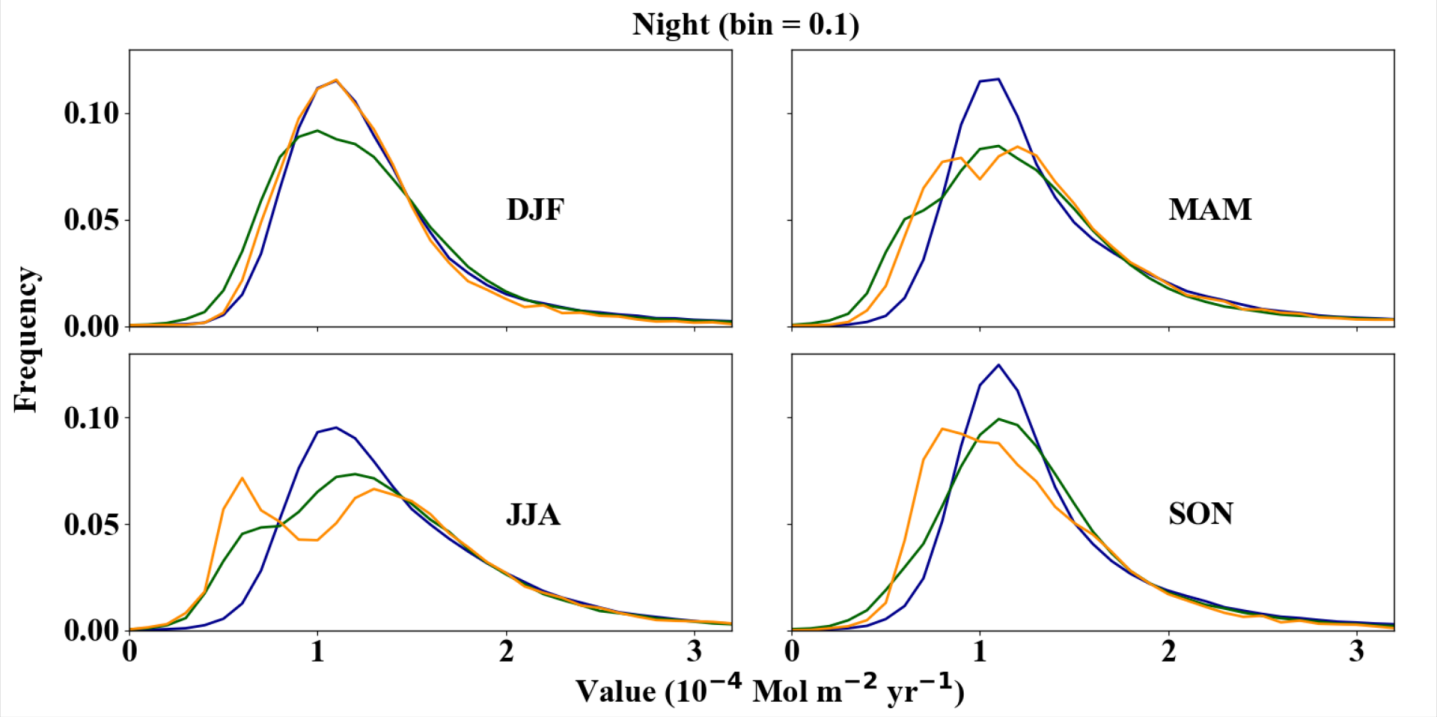






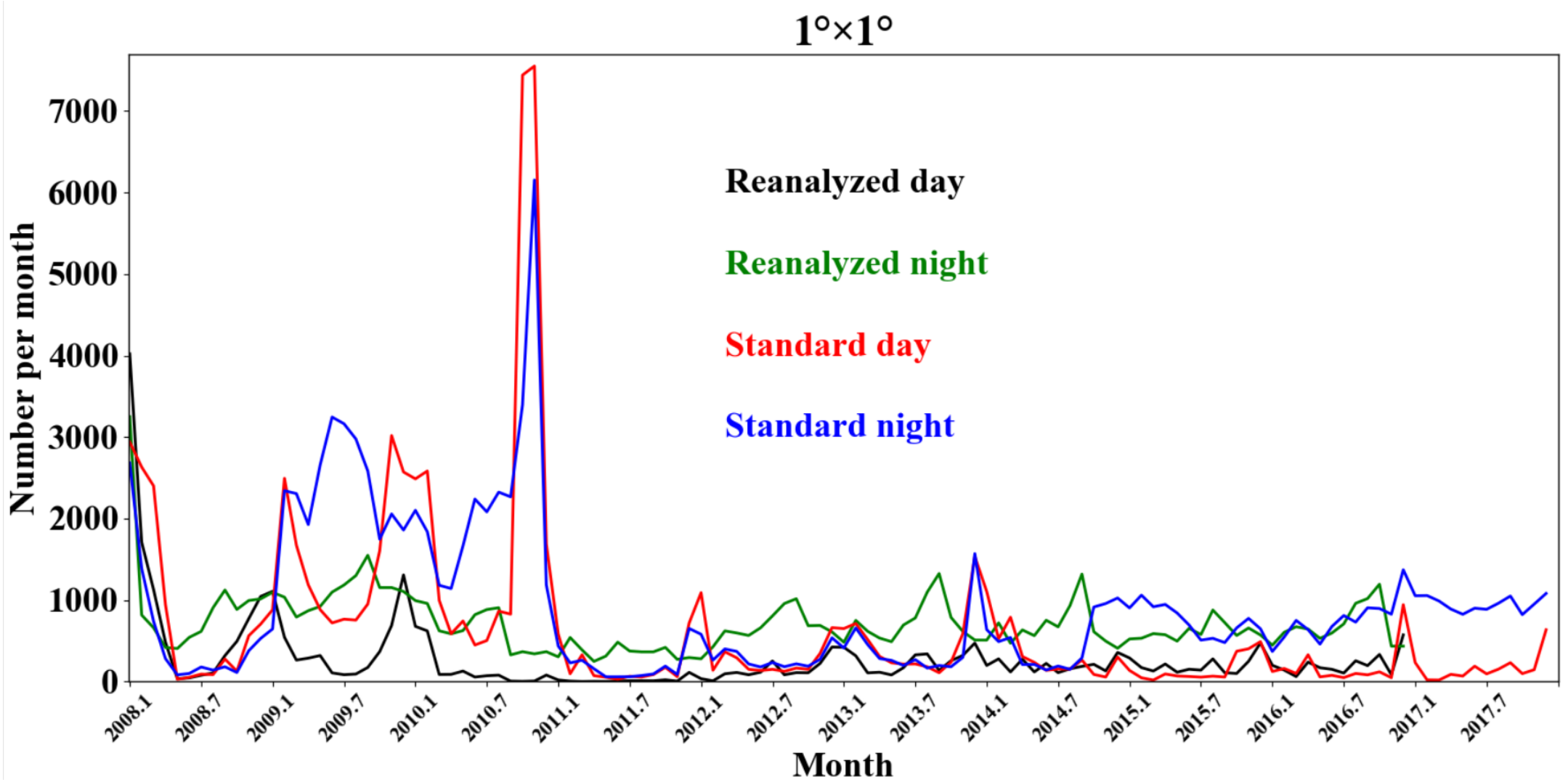
Seasonal trend in the equivalent latitude over 2008-2016 (day and night)





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

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



End