Minimizing sampling biases in SAGE III/ISS and merged multi-satellite ozone datasets

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Development and utilization of multi-sensor ozone data record for long term trend studies and model evaluations

Outline

- Motivations
- Update on SAGE III/MLS ozone comparisons
- Sampling biases in non-uniform satellite measurements (i.e. SAGE III/ISS) derived climatologies
- Methodology to correct/reduce sampling biases
- Results
- Conclusions and future works

Introduction (Motivations)

- Research questions: How is atmospheric composition changing? How will future changes in atmospheric compositions affect ozone, climate and global air quality?
- In previous studies there are inconsistencies between satellite observed and chemistry-climate model (CCM) predicted lower stratospheric ozone trends since late 1990s/2000 (e.g. Ball et. al., 2018, 2020; SPARC/IO3C/GAW, 2019)
  - CCM simulations indicate decreasing ozone trends in the tropical lower stratosphere and increasing ozone trends in the mid-latitude lower stratosphere (mainly result from increasing GHGs and enhanced BDC)
  - Observations from merged satellite data records, however, show negative ozone trends in mid-latitude lower stratosphere
- Inconsistencies could result from (a) uncertainties in merged satellite datasets, and/or (b) deficiencies in CCMs such as lacking realistic dynamic transport

Introduction (Motivations)

- Uncertainties in merged satellite data sets
  - It's common to use derived climatologies (monthly zonal means) from merged satellite data records (e.g. GOZCARDS, SWOOSH) for ozone trend studies
  - Inhomogeneous sampling in space and time, however, can introduce significant biases (>5-10%) in calculated climatologies (e.g. monthly zonal means) from satellite measurements (Toohey et al., 2013)
  - The sampling biases can lead to ~1%/decade in derived ozone trends if not properly accounted for (Damadeo et al., 2018)
- Proposed task: Investigate and minimize sampling biases in merged satellite data records (GOZCARDS), some results will be shown in this presentation later

Introduction (Motivations)

- Possible deficiencies in CCMs
  - There are several competing mechanisms affecting ozone trends in the lower stratosphere and upper troposphere, for example
  - The response of Brewer Dobson circulation (BDC) to changing greenhouse gases (GHGs) vs ozone depleting substances (ODSs)
  - The response of mid-latitude lower stratospheric ozone to downward transport vs isentropic mixing of BDC
  - Other short term (inter-annual) dynamic variabilities

Brewer Dobson circulation and the distribution of ozone

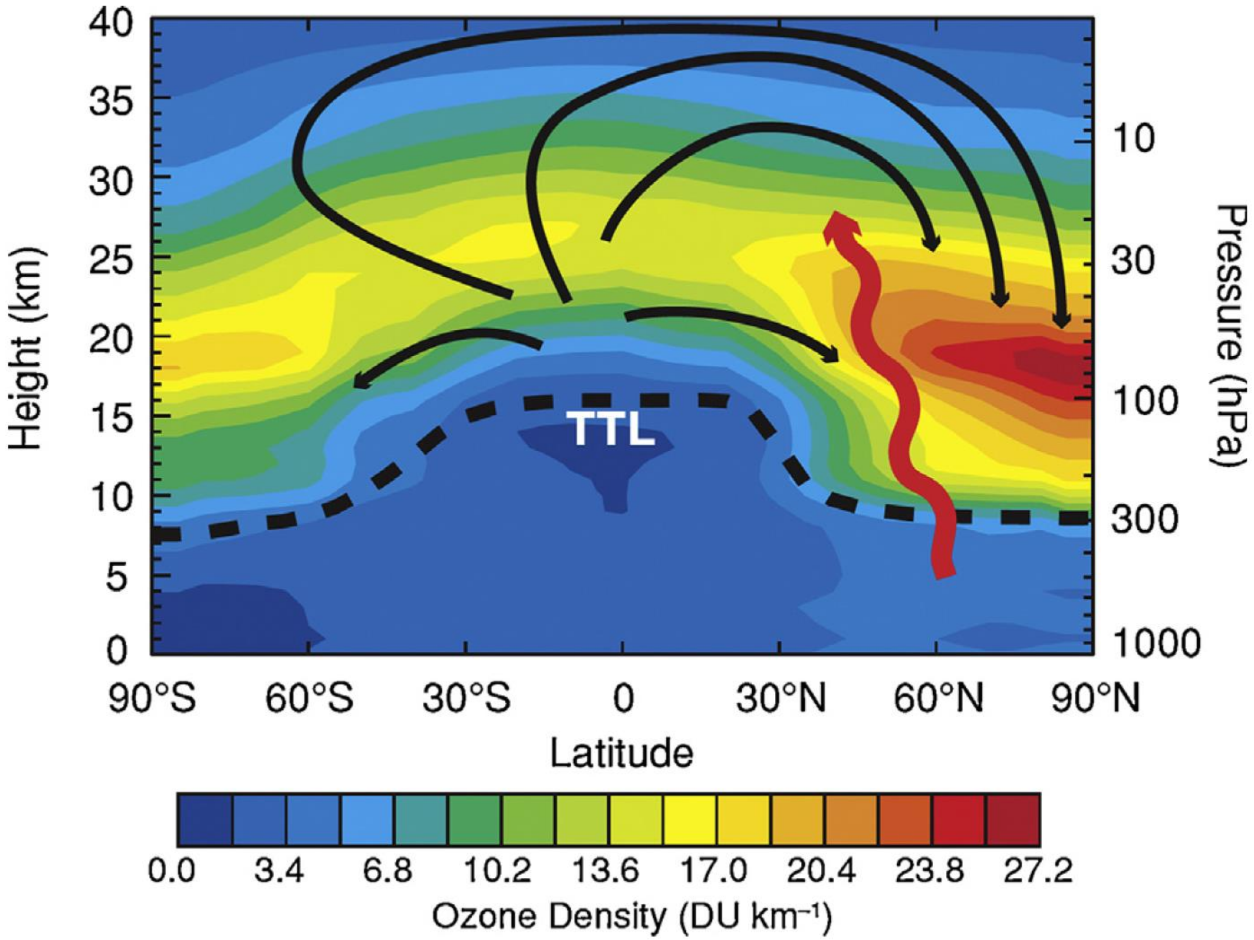


Figure from Jacobs (2014)

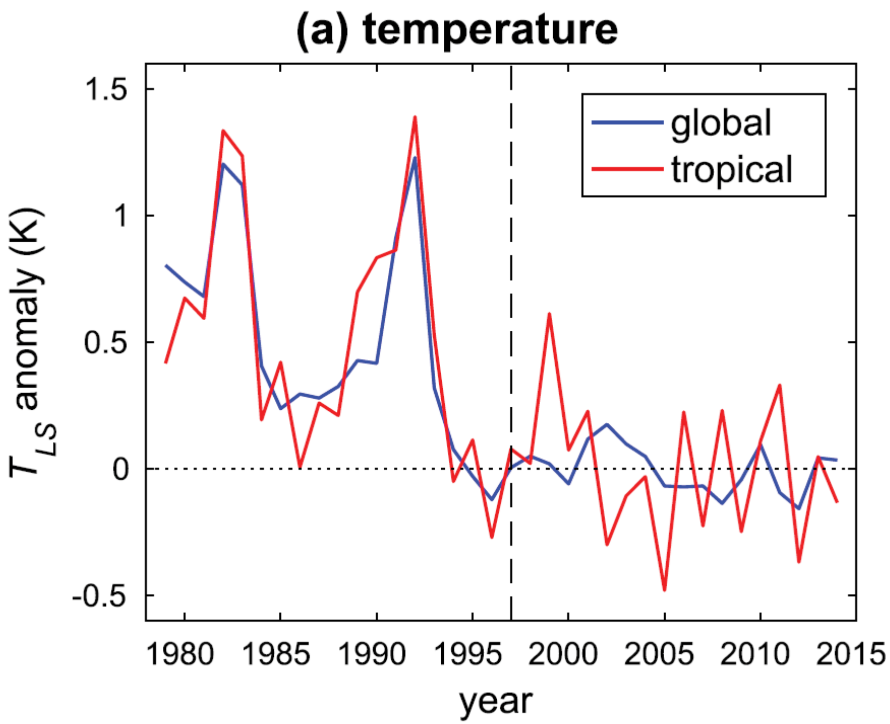
BDC during the northern hemisphere winter

Greenhouse gases (GHGs) (e.g. CO2) increase can enhance the BDC (e.g. Butchart, 2014)

descending: bring ozone rich air to mid-latitude LS

Isentropic mixing: bring ozone poor air from the tropics to mid-latitude LS

Observed temperature and ozone anomalies in the tropical lower stratosphere (1979-2014)



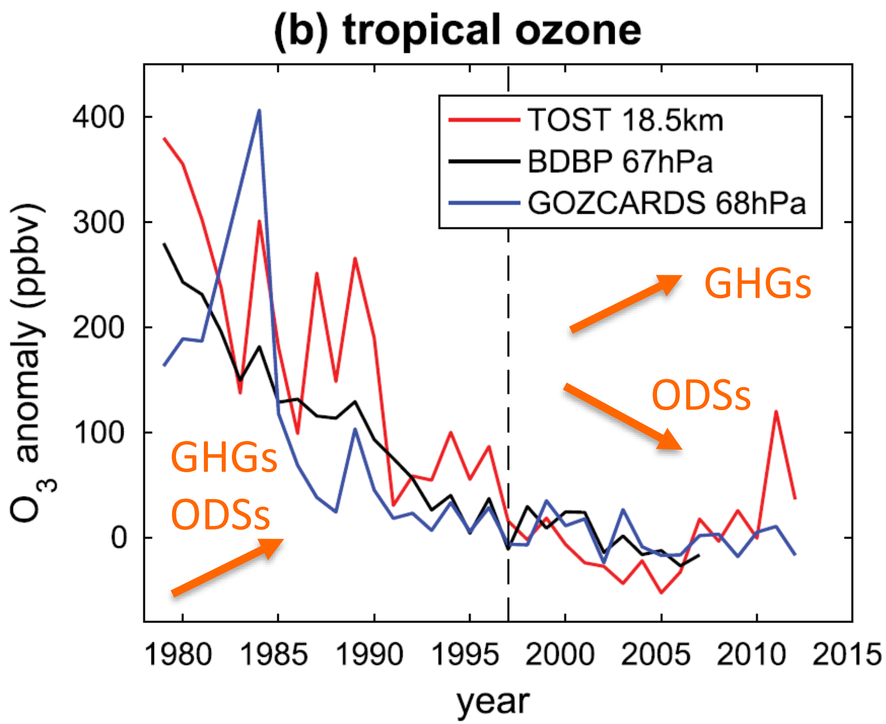


Figure from Polvani et al., 2017

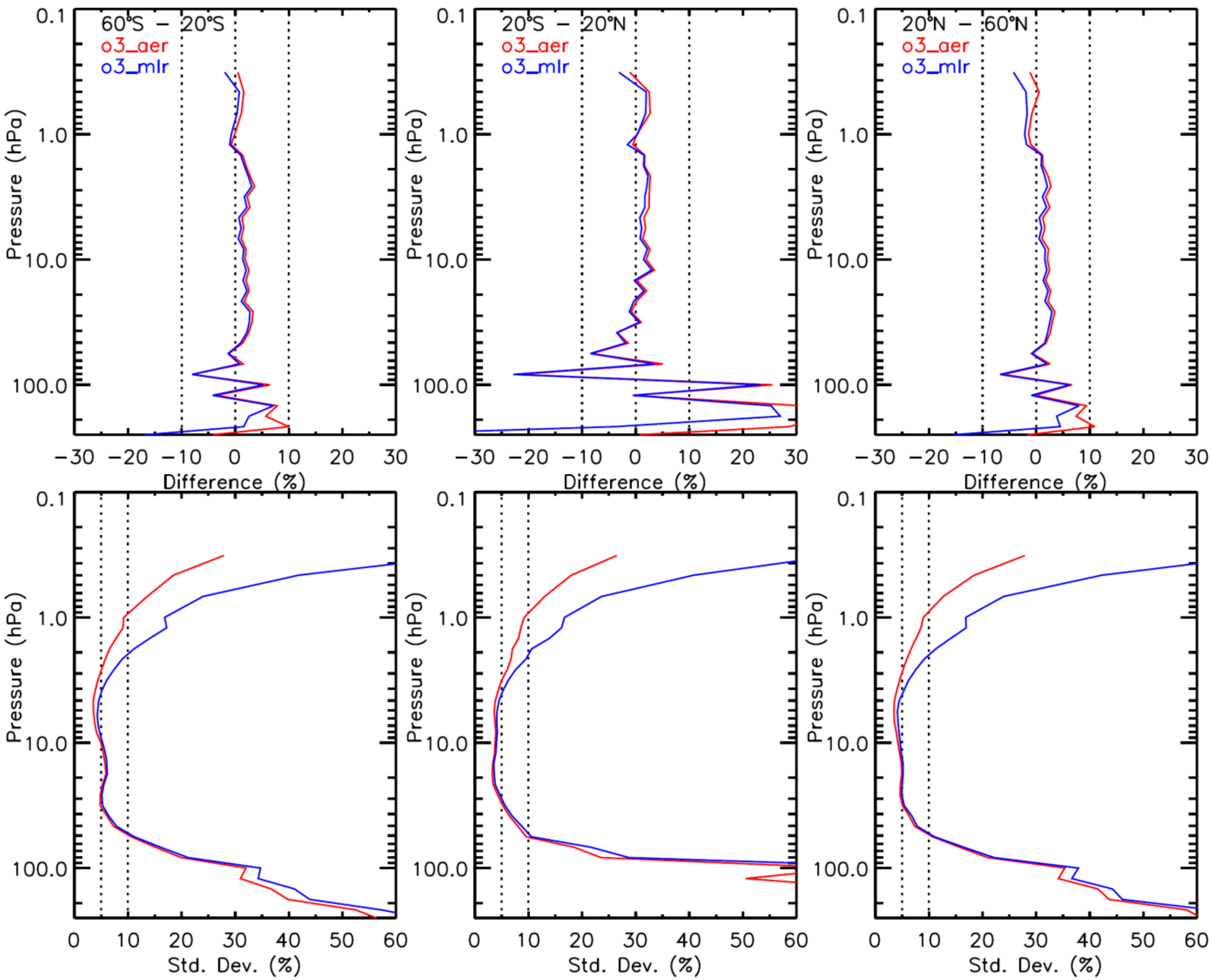
Flattening pf temperature and ozone trends in the tropics after late 1990s indicates weakening of Brewer Dobson Circulation due to decreasing ODS

How BDC reacts to increasing GHGs and decreasing ODSs in CCM?

Introduction (Motivations)

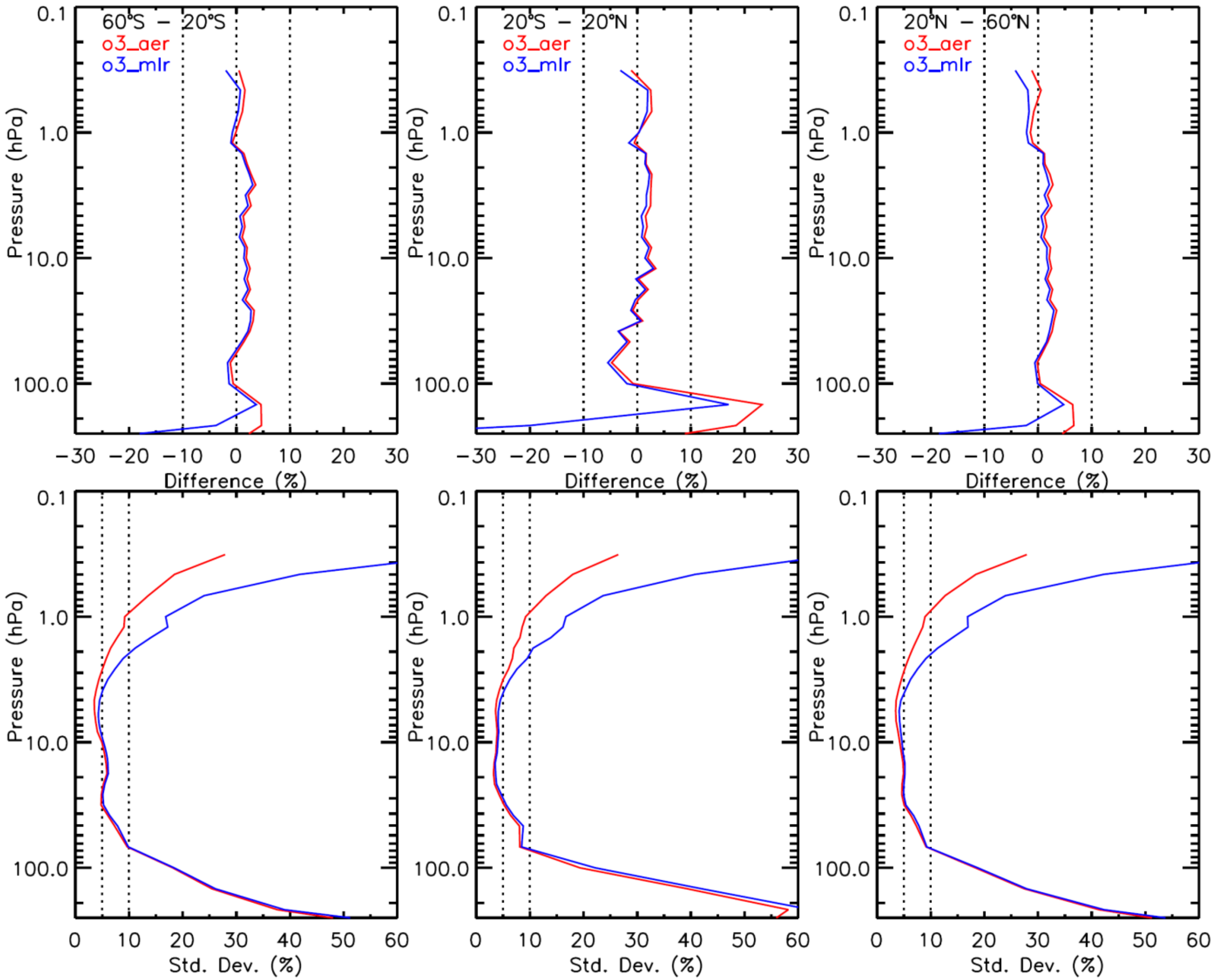
- Possible deficiencies in CCMs
  - There are several competing mechanisms affecting ozone trends in the lower stratosphere and upper troposphere, for example
  - The response of Brewer Dobson circulation (BDC) to changing greenhouse gases (GHGs) vs ozone depleting substances (ODSs)
  - The response of mid-latitude lower stratospheric ozone to downward transport vs isentropic mixing of BDC
  - Other short term (inter-annual) dynamic variabilities
- Proposed tasks: use SAGE (merged) satellite data and other correlative data (ozone sondes) and model (GMI-CTM) to better understand and attribute observed ozone trends, and differences between observations and CCMs simulations.
  - Ozonesondes related studies, see Ann Thompson’s presentation
  - Model related studies (Susan Strahan) will be presented in future meetings

Comparisons of SAGE III/ISS (V5.2) and Aura MLS (V5.x) ozone (6/2017-8/2021)



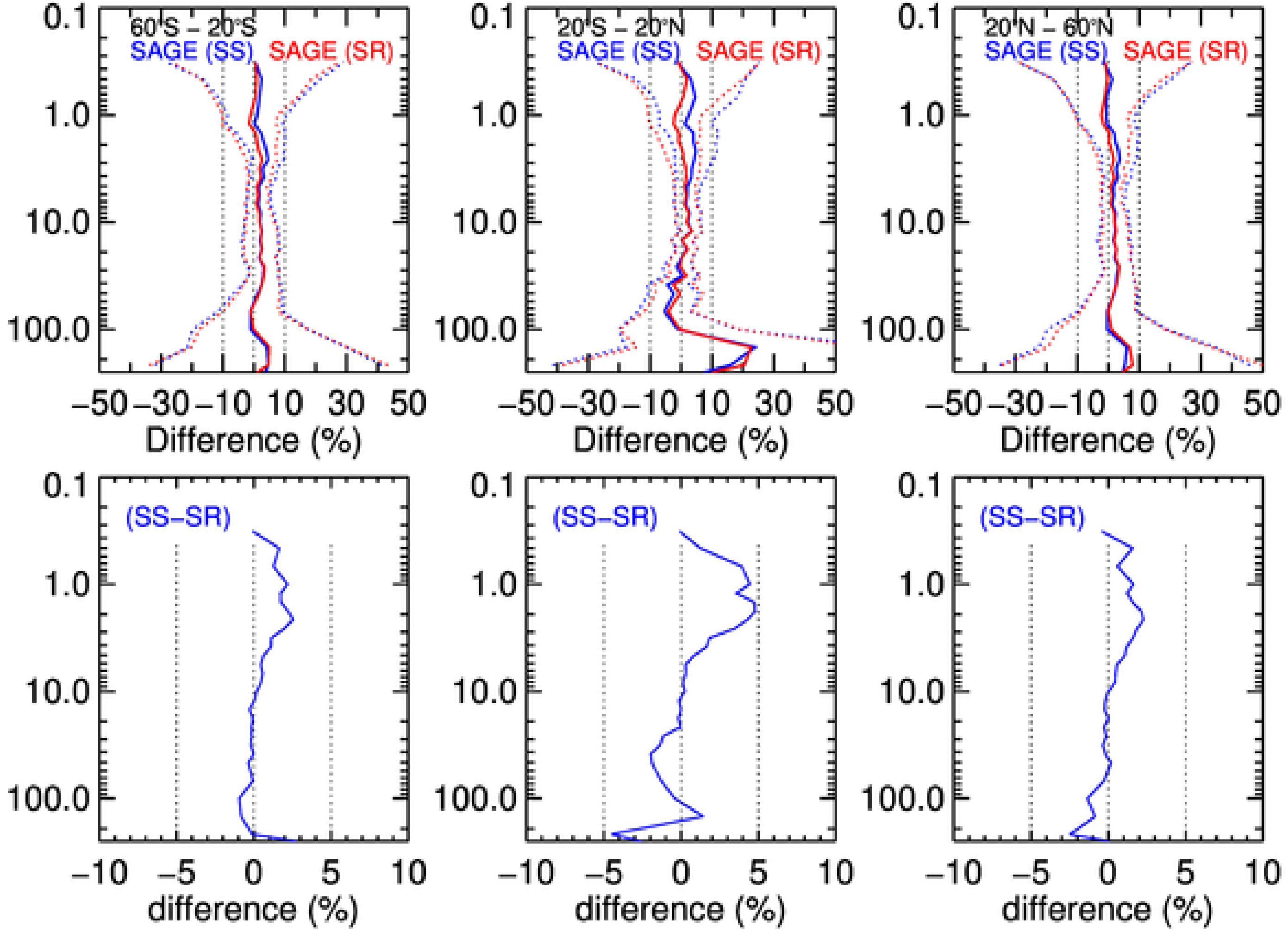
- SAGE III (v5.2) and MLS (v5.x) ozone show very good agreements (within 2-3%) for most of stratosphere.
- In the lower stratosphere the SAGE/MLS differences show oscillation with altitudes features, which mainly result from artifacts in MLS retrievals (vertical resolution)

Comparisons of SAGE III/ISS (V5.2) and Aura MLS (V5.x) ozone (6/2017-8/2021)



- MLS ozone below 46 hPa were smoothed to (1000./$10^{i/6}$) levels (twice of reported vertical resolution).
- SAGE III and MLS ozone show very good agreements in the stratosphere, within 2-3% down to ~5 km above tropopause; and ~5% near tropopause
- SAGE III MLR (v5.2) ozone retrieval in lower stratosphere is greatly improved

SR/SS differences in SAGE III/ISS (V5.2) ozone (use MLS as transfer standard)

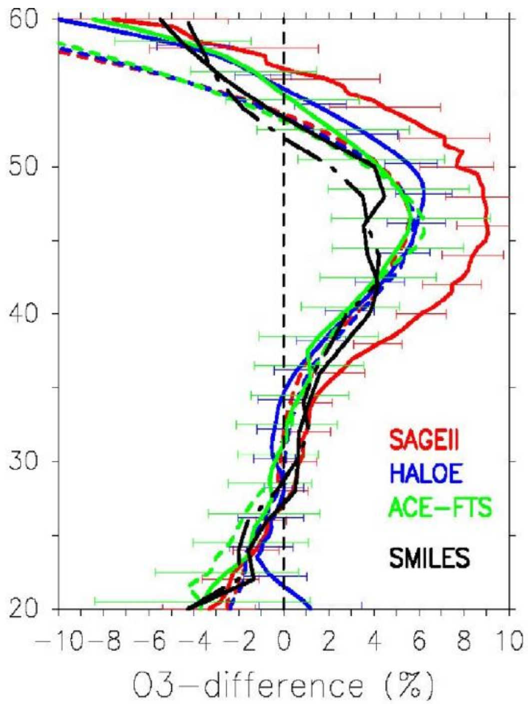


SR/SS differences are reduced in v5.2 (consistent with other measurements and WACCM model)

SR/SS differences in SAGE retrieved ozone

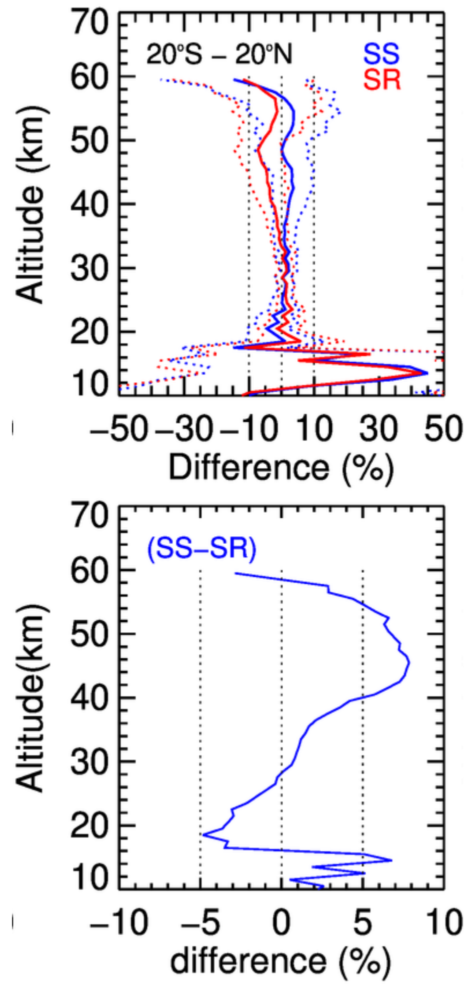
SAGE II

(SS-SR) differences
10°S-10°N,

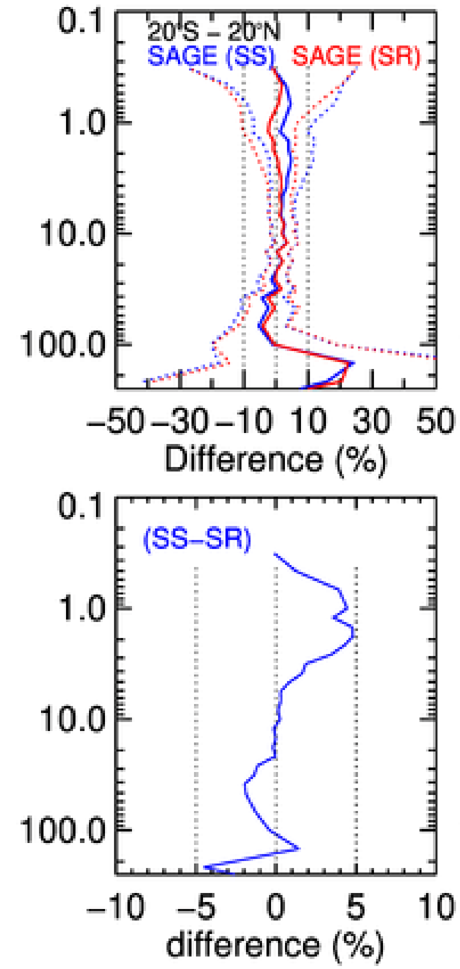


(Sakazaki et al., 2015)

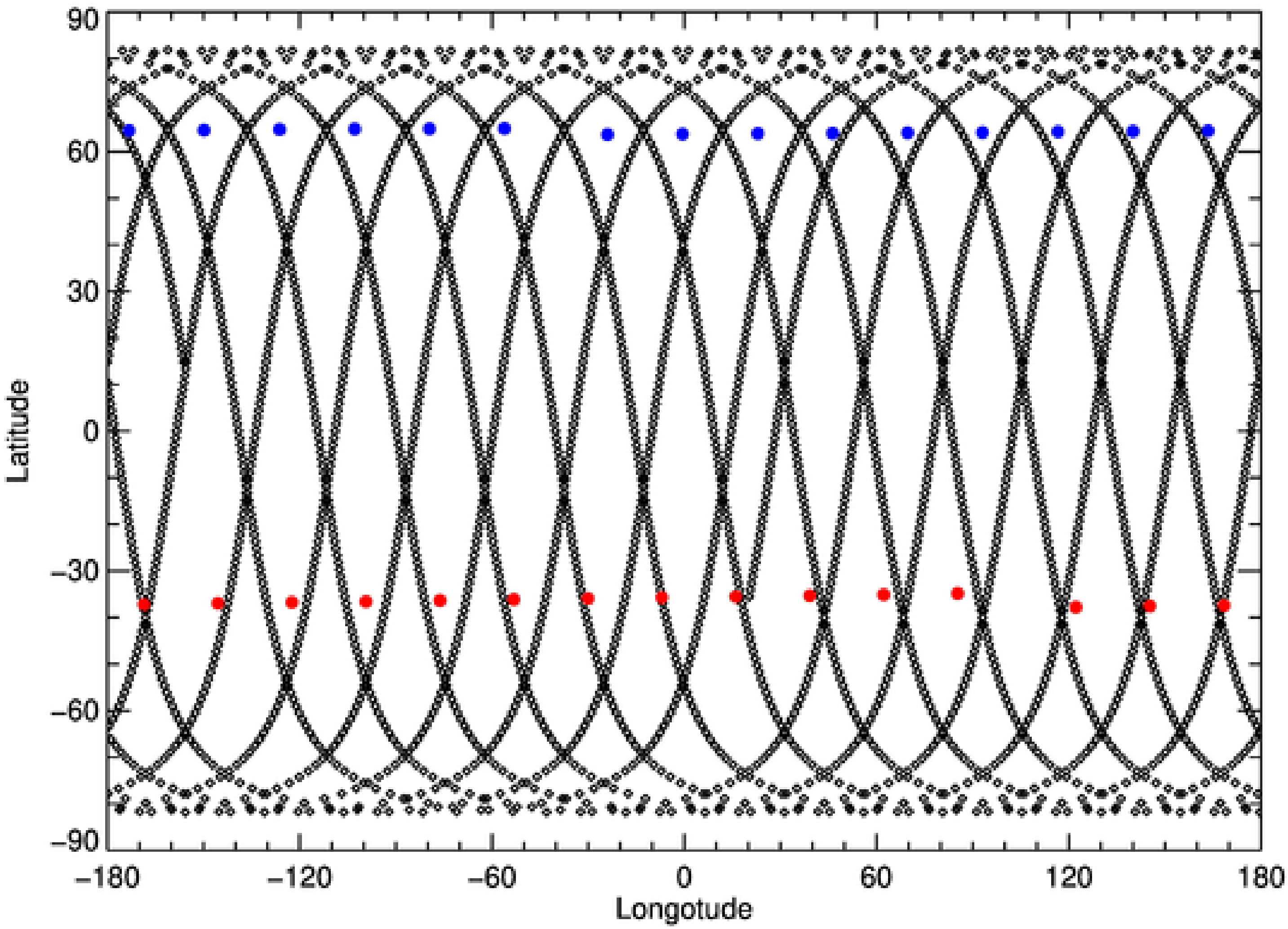
SAGE III/ISS (v5.1)



SAGE III/ISS (v5.2)

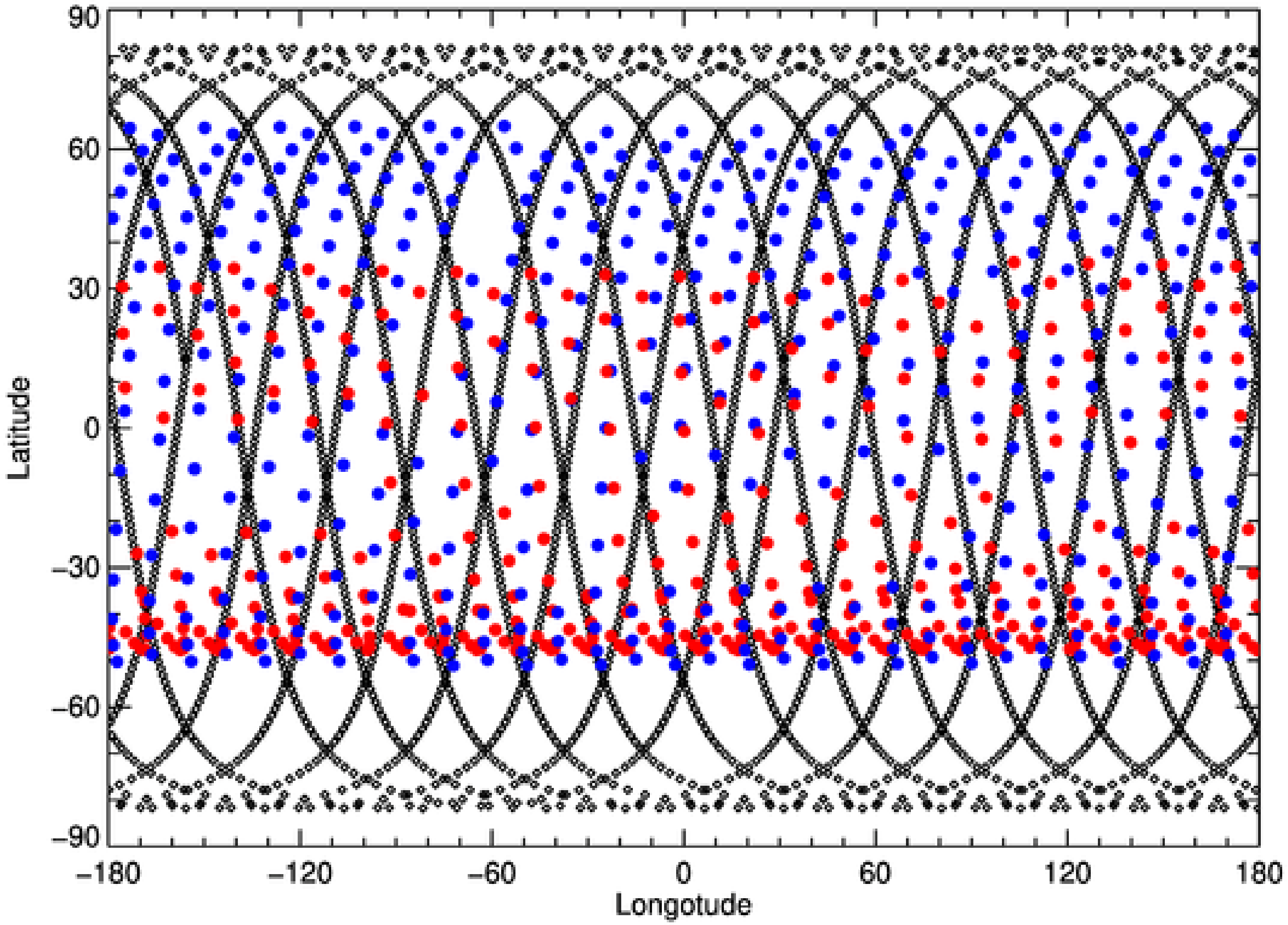


An example of SAGE III/ISS and Aura MLS observed locations on Aug. 1, 2017



AMLS
SAGE SR
SAGE SS

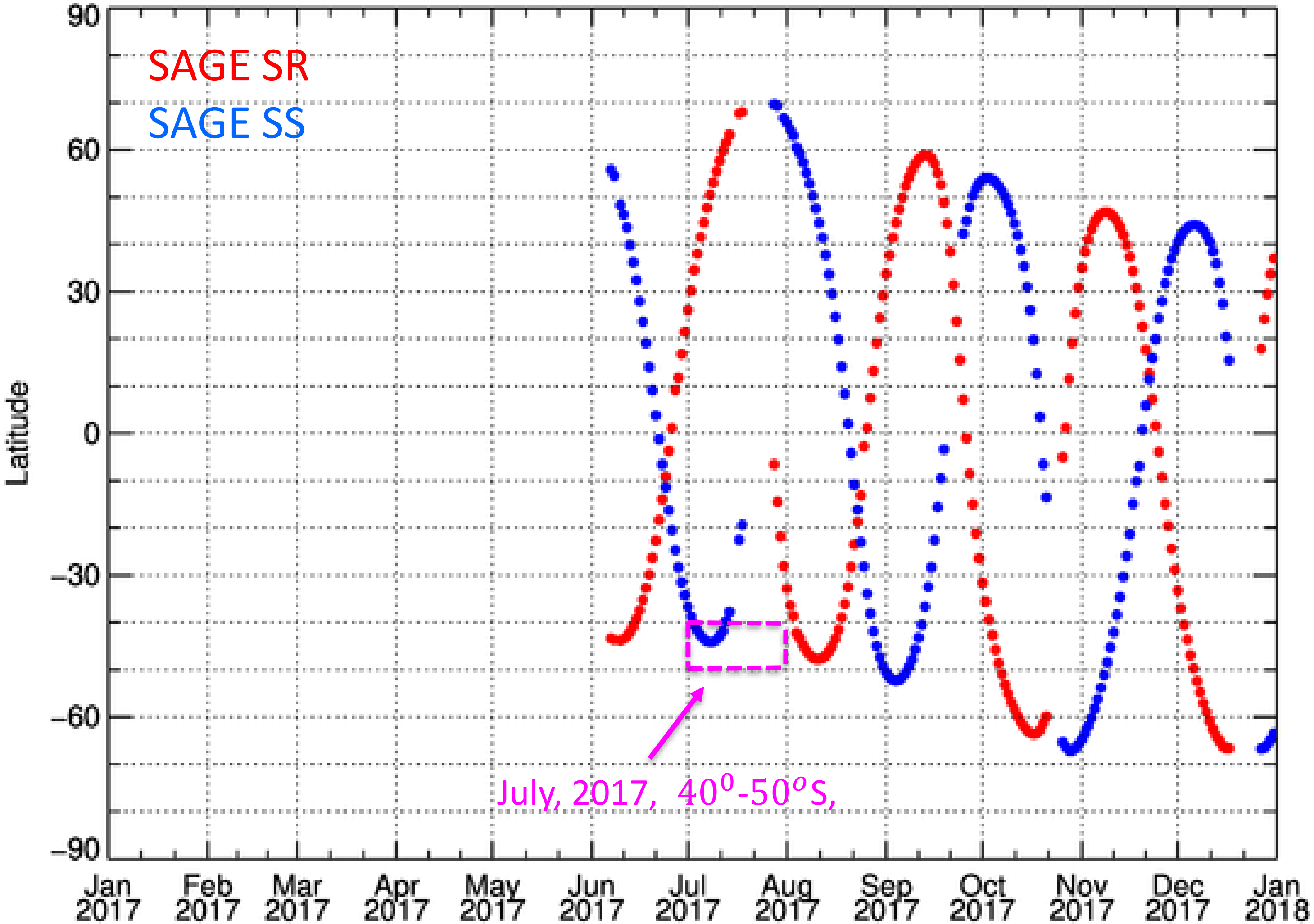
All SAGE III/ISS observed locations in Aug. 2017



SAGE SR
SAGE SS

For clarification only one day of AMLS measurements (Aug. 1, 2017) are shown

Daily mean latitudinal coverages of SAGE III/ISS observations in 2017



Non-uniform measurements in space, time, or event type (sr/ss) could result in sampling biases in derived MZM

Sampling Bias Estimation

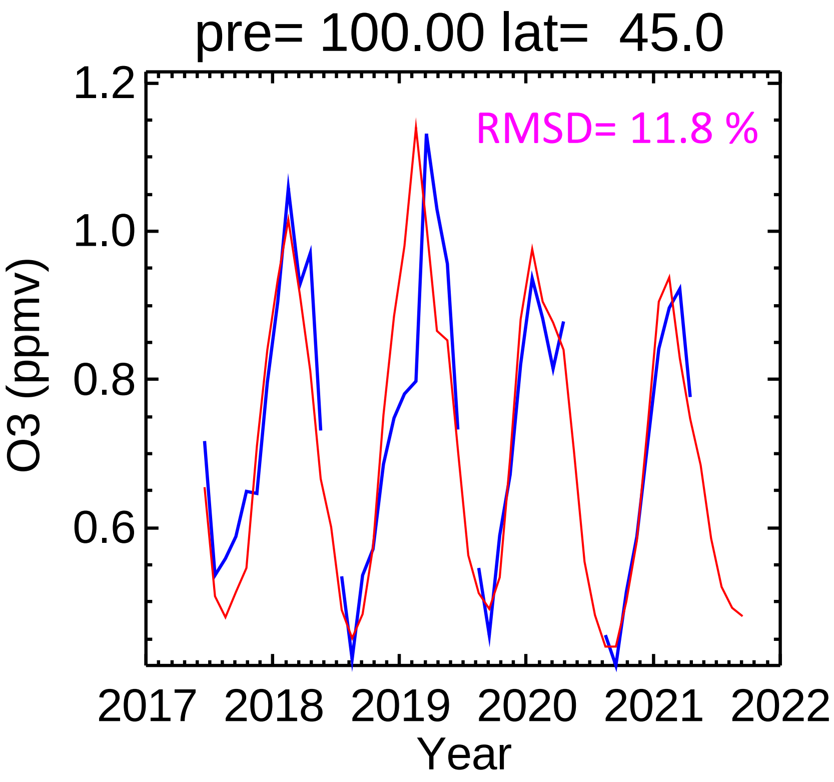
- Use Aura MLS O3 data (from 6/2017 to 7/2021) to calculate the "true" MZM.
- Choose subsampled MLS data with SAGE observed locations/times
  - (i.e. <1^0 latitude, $< 8^0$ longitude, night time)
  - choose the closest one in distance if there are more than one MLS profile collocated with each SAGE profile.
- Calculate the MLS monthly zonal means (MZM) at each 10 degree latitude bin based on original samplings and sub-sampled with SAGE's locations
- The estimated sampling bias is calculated by root mean square difference (RMSD)

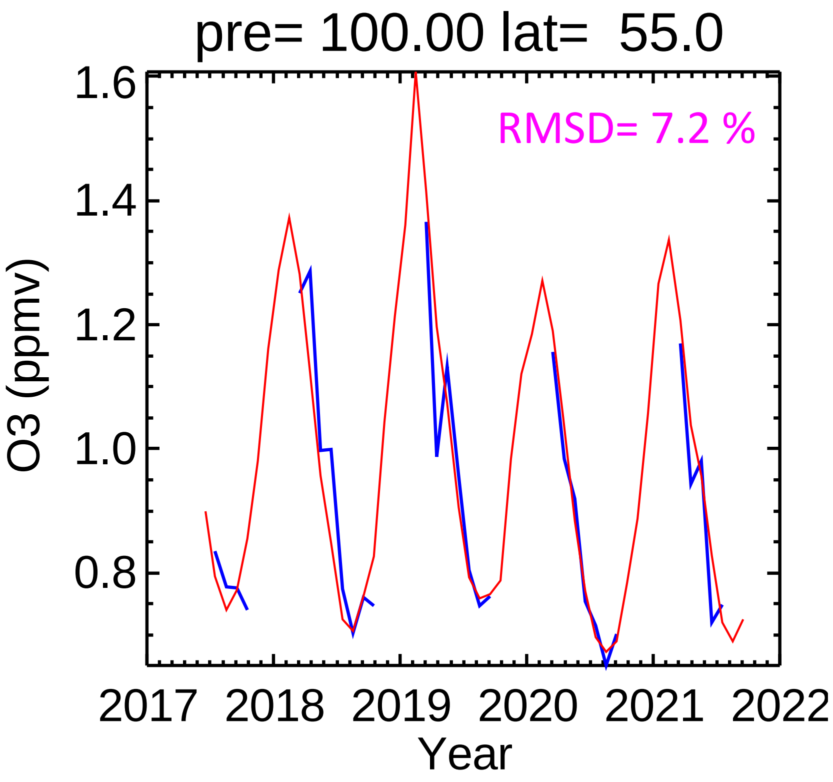
$$Bias = \sqrt{\frac{\sum_{i=1}^{N}\left(\frac{x(s)_i - x(o)_i}{x(o)_i}\right)^2}{N}}$$

X(s), MZM with SAGE samplings
X(o), MZM with MLS samplings
N, total number of months

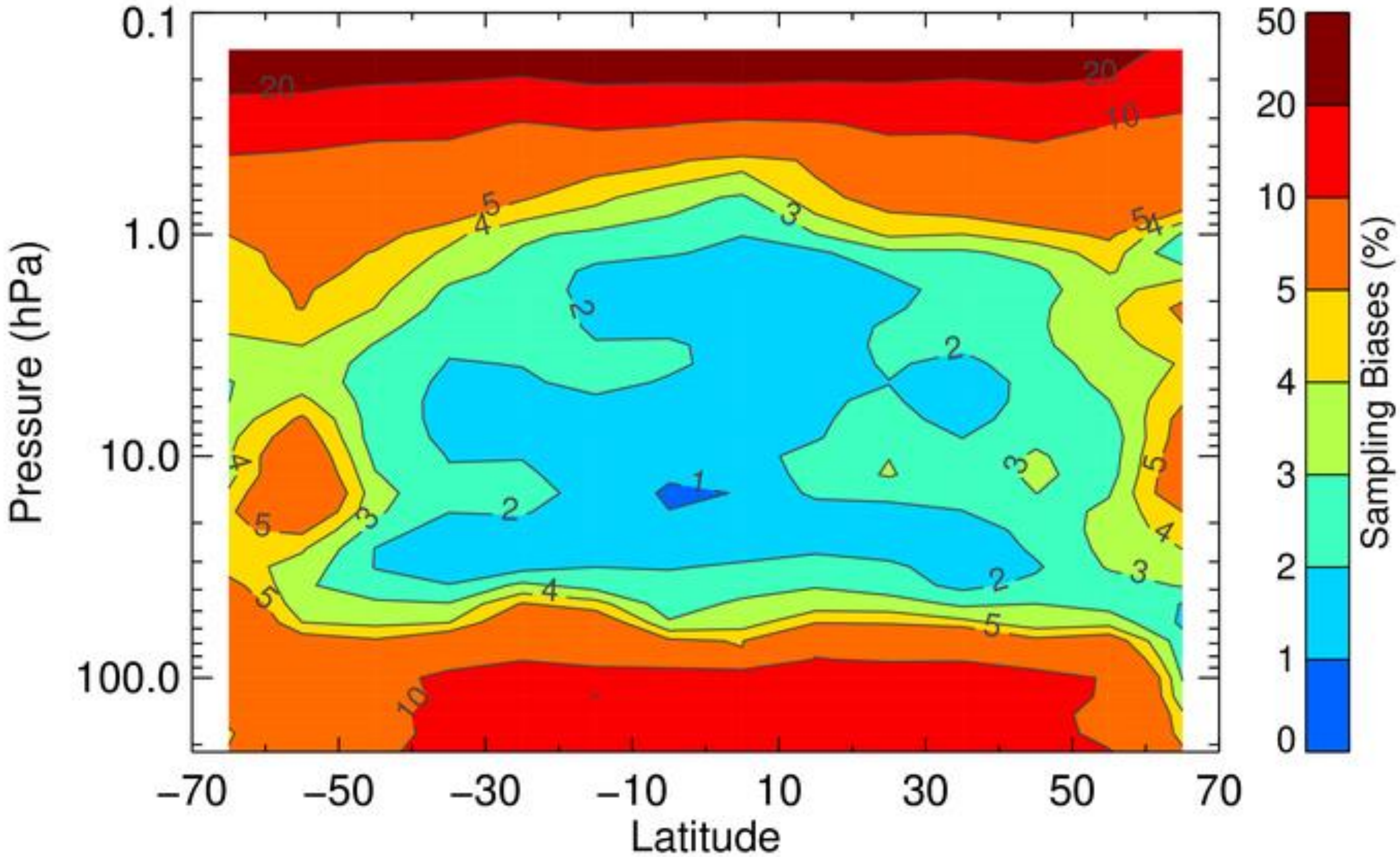
Examples of Aura MLS monthly zonal mean ozone based on different samplings

original sampling;   subsampled with SAGE III/ISS locations/times





Estimated sampling biases (RMSD) in Aura MLS MZM ozone based on SAGE III/ISS sampling pattern



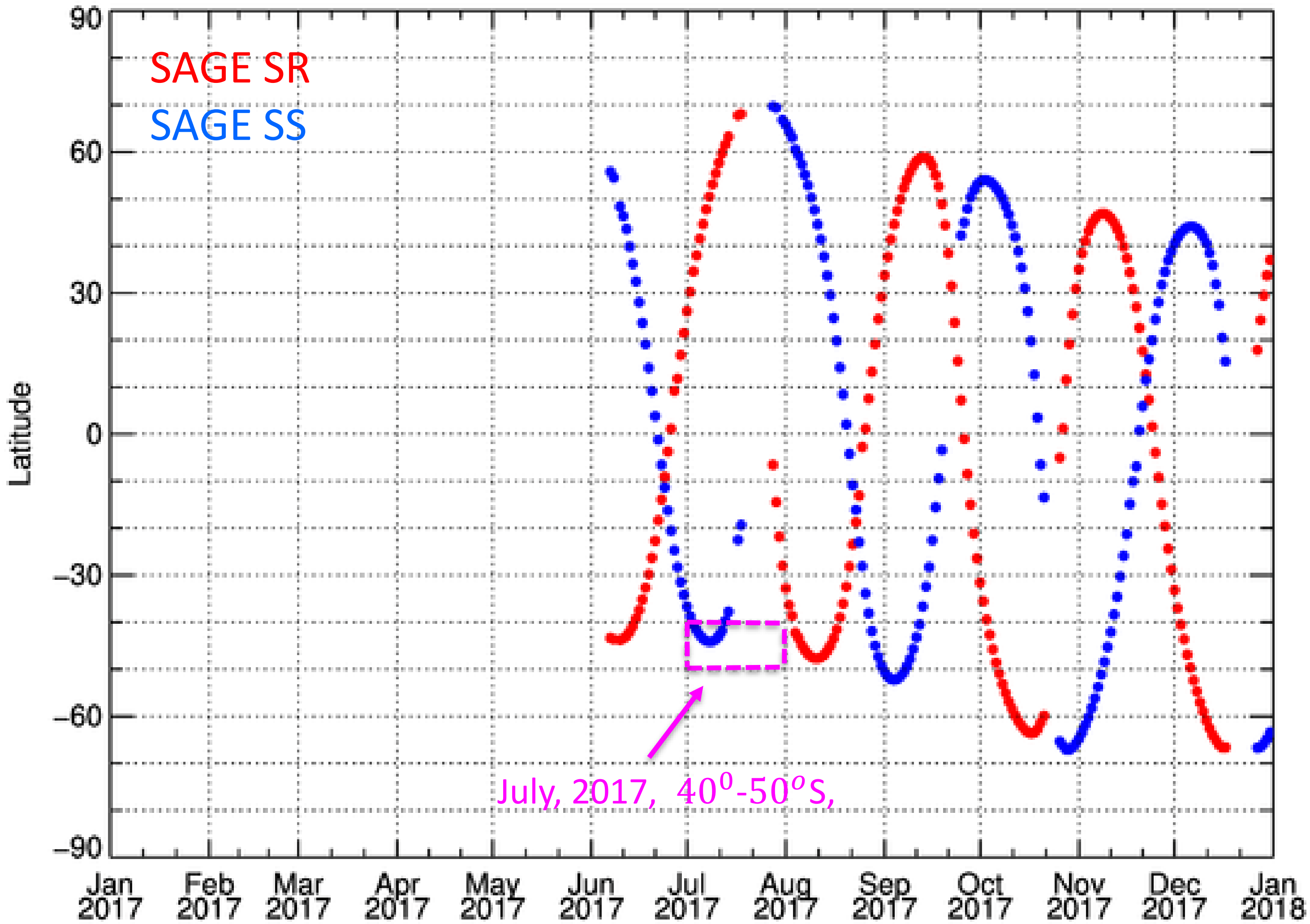
Use data between 6/2017 and 7/2021

- Sampling bias of 1-3% can be seen in most of the stratosphere between 50 N and 50 S and for altitudes above ~40hPa

- Larger sampling biases (5-10%) can be found in high latitude stratosphere and in the UT/LS
- The large sampling biases in mesosphere mainly result from diurnal cycle

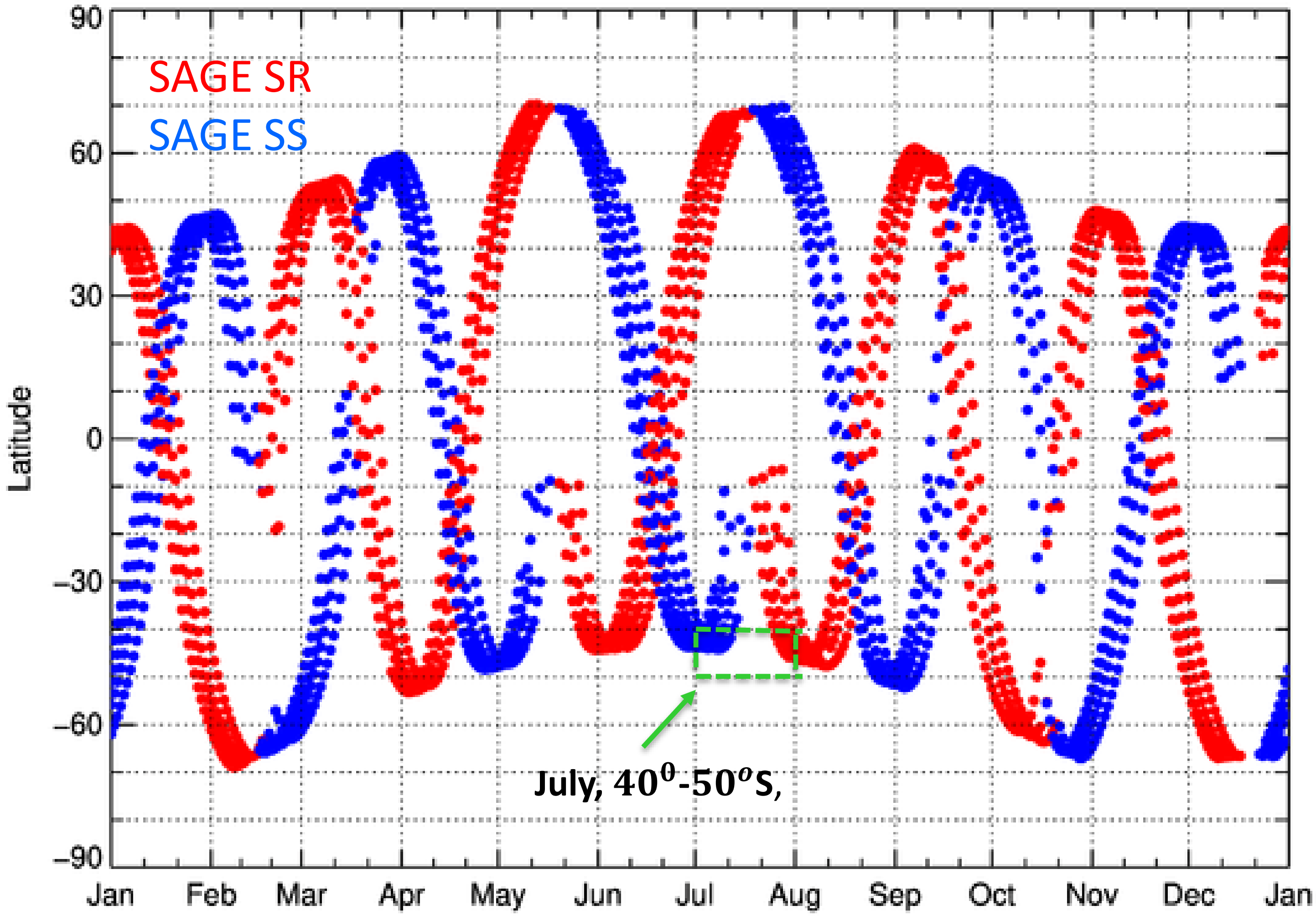
- How to correct (minimize) sampling biases in derived monthly zonal mean values?
- Two dimensional regression models had been used to infer long term ozone trends (e.g. Bodeker et al., 2013; Damadeo et al., 2014)
  - Imply the spatial-temporal evolution of ozone can be better characterized by 2-D regression model
- Investigate whether we can use 2-D regression model to adjust (minimize) sampling bias in SAGE (and other non-uniform satellite measurements)
- Quantify the effect of sampling bias adjustment

Daily mean latitudinal coverages of SAGE III/ISS observations in 2017



To better characterize the spatial-temporal variations within a month/latitude band, use multi-year daily mean values, instead of monthly zonal means

Daily mean latitudinal coverages of SAGE III/ISS observations between 6/2017 and 7/2021



daily zonal mean latitudes as a function of day of year

Daily zonal mean ozone extend across different time and latitude within a specific month and latitude band can be used to characterize the spatial-temporal evolution of ozone in that month and latitude band

Regression model to characterize ozone variations in time (and space)

- An example of traditional (1-D) regression model (no EESC, Pinatubo terms) based on monthly zonal mean (MZM)

$$\overline{M}(t) = \sum_k \beta_k T_k(t) = \beta_0 + \beta_1 S(t) + \beta_2 T(t) + \beta_3 QBO(t) + \beta_4 Solar(t) + R(t)$$

- Two dimensional regression model based on daily zonal mean

$$\overline{D}(\theta, t') = \sum_i \sum_k \beta_{i,k} \Theta_i(\theta) T_k(t')$$

$$= \sum_{i1} \beta_{i1} \mathrm{P}_{i1}(cos\theta) + \sum_{i2} \beta_{i2} P_{i2}(cos\theta) S(t') + \sum_{i3} \beta_{i3} \mathrm{P}_{i3}(cos\theta) T(t')$$

$$+ \sum_{i4} \beta_{i4} \mathrm{P}_{i4}(cos\theta) QBO(t') + \sum_{i5} \beta_{i5} \mathrm{P}_{i5}(cos\theta) Solar(t') + R(t')$$

notes: $\mathrm{P}_i(cos\theta)$: *Legendre polynomial*; t': *day of yeaar*

References: Bodeker et. al., (2013); Damadeo et al., (2014)

Sampling Bias Adjustment

The following procedures are used to adjust sampling biases

- At each altitude apply 2-D regression model to all subsampled MLS daily mean data (e.g. all available data between 90S and 90N, instead of at particular latitude band).
- Use regression model results to adjust original data (before deriving MZM)

$$\bar{D}(\theta,t)_{adj} = \bar{D}(\theta,t)_{org} \times \frac{\bar{D}_p(\bar{\theta},\bar{t}\,)}{\bar{D}_p(\theta,t)}$$

$\bar{D}(\theta,t)_{org}$, $the\ daily\ mean\ at\ latitude\ \theta, and\ time\ t\ (day\ of\ year)$

$\bar{D}_p(\theta,t), model\ predicted\ daily\ mean\ at\ original\ latitude(\theta), and\ time\ (t)$

$\bar{D}_p(\bar{\theta},\bar{t}\,), model\ predicted\ temporal - zonal\ mean\ at\ mean\ latitude(\bar{\theta}), and\ mean\ time\ (\bar{t}\,)$

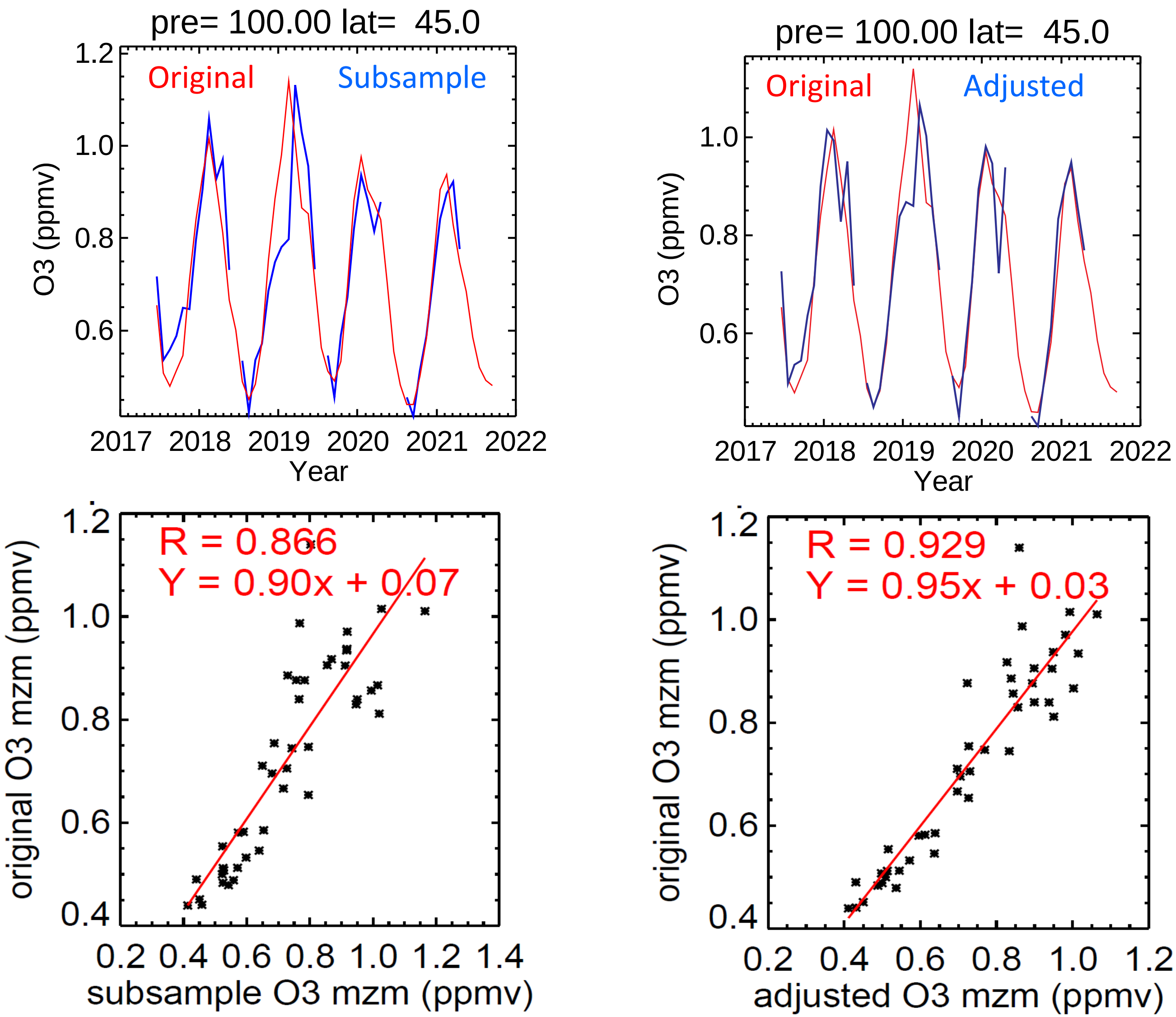
Similar technique can be found in Kloss et al. (2019) for ACE-FTS carbonyl sulfide

Sampling Bias Adjustment

Notes for regression model used in this study

- Use seasonal cycle, trend, and QBO terms only in the model
- Use 7 terms Legendre Polynomials ($P_i(cos\theta)$, i = 0 to 6)
- Seasonal Cycle is represented by two Fourier pairs (i.e. with 12 month and 6 month period)
- QBO term is represented by the fist four principal components of Singapore winds (i.e. apply principal component analysis (PCA) for Singapore winds at 7 pressure levels, from 10 to 70hPa)
- The number of terms for Legendre polynomial, seasonal and QBO terms are tunable, and it could be different based on different studies.

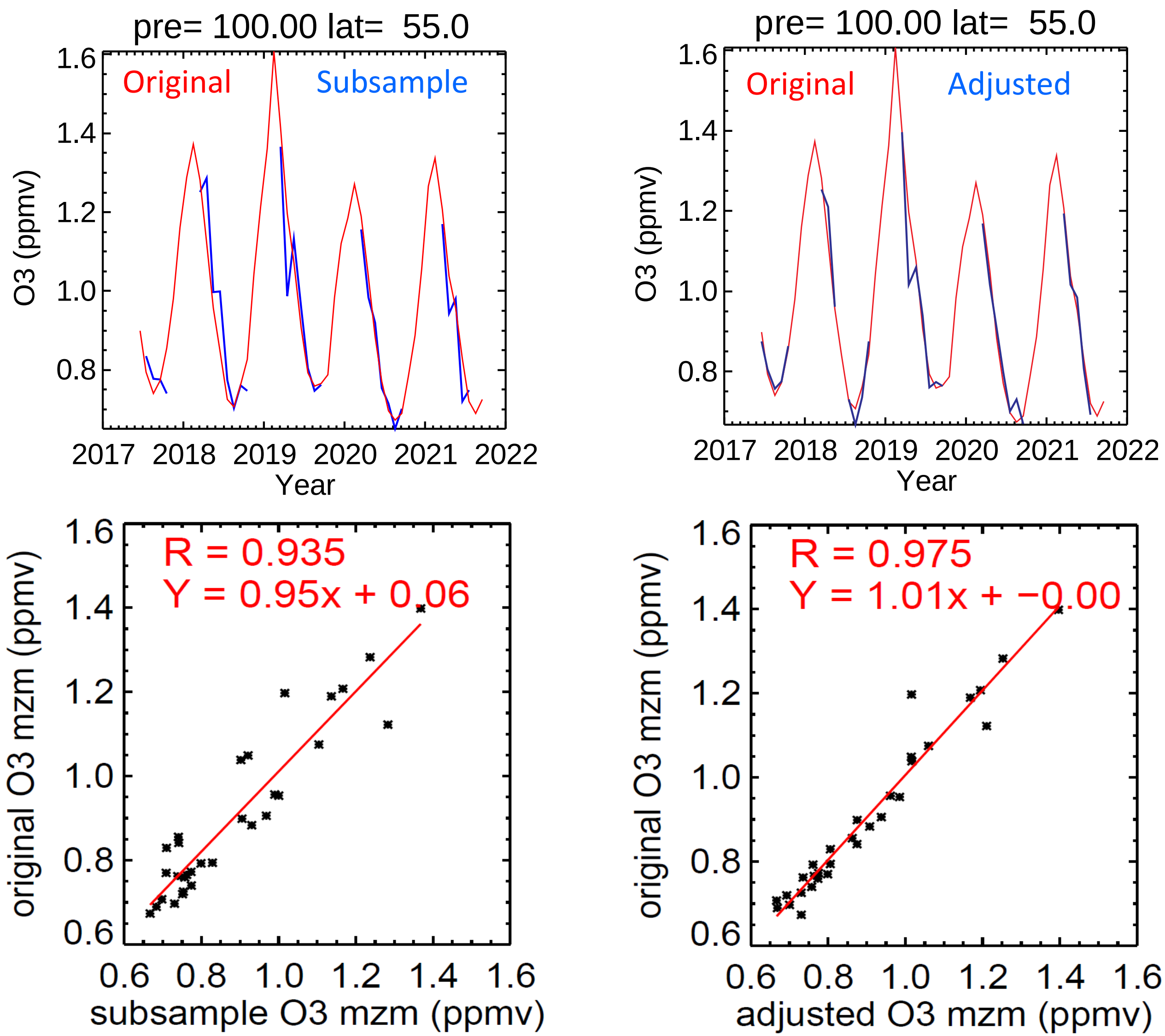
Comparisons of subsampled Aura MLS MZM ozone with and without sampling bias correction



at 100 hPa, 40^o-50^o N

Compared to subsampled (unadjusted) measure-ments, the sampling-bias adjusted monthly zonal mean shows better agreement with original MLS data (i.e. with smaller RMSD and larger linear correlation).

Comparisons of subsampled Aura MLS MZM ozone with and without sampling bias adjustment

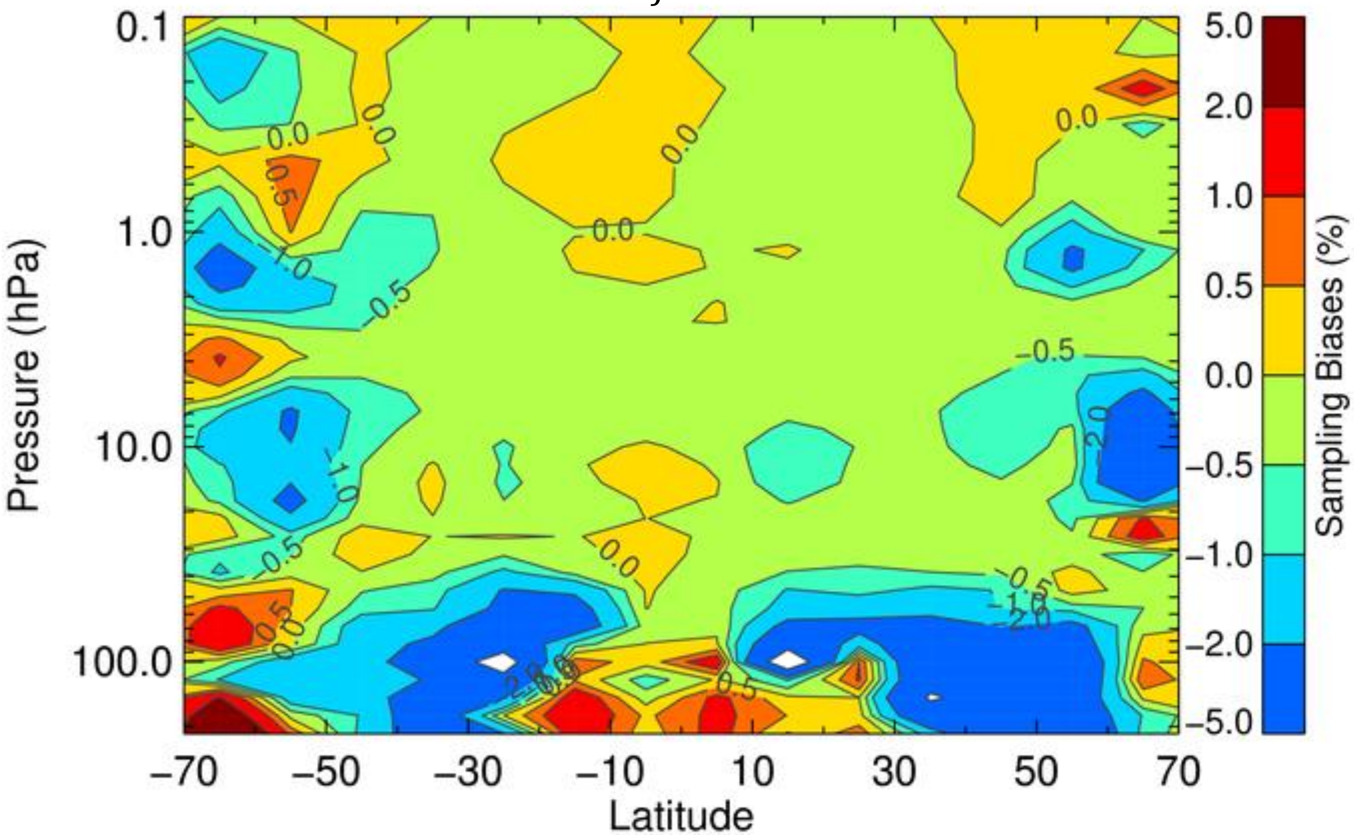


at 100 hPa, 50^o-60^o N

Reduce scattering along the regression line

Reduction of sampling bias after applying corrections to subsampled MLS ozone data

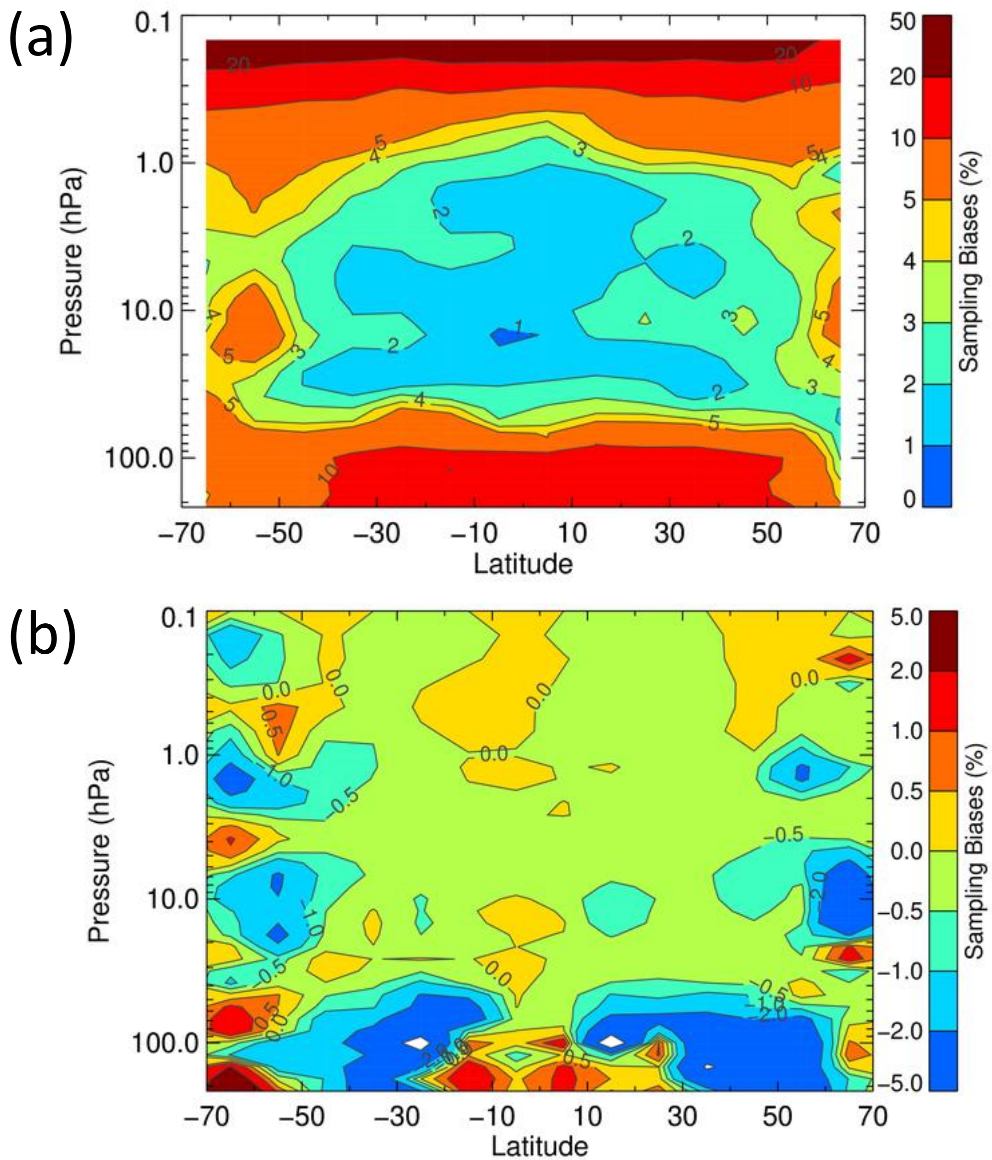
$Bisa_{adj} - Bias_{sub}$



Negative values indict reduction of sampling bias after applying sampling bias adjustment.

Positive values indicate increase of sampling bias after applying sampling bias adjustment

The estimated sampling bias in SAGE III/ISS MZM ozone (a) and the effect of correction on estimated sampling bias (b)



The sampling biases in SAGE III MZM can be reduced by 1-5% (from 5-10%) in the subtropical and mid-latitude UT/LS regions by applying corrections/adjustments (this is the regions where CCMs and merged satellite datasets show inconsistent ozone trends after late 1990s/2000).

Conclusions and future works

- The SAGE III/ISS (v5.2) solar ozone show very good agreements with Aura MLS (v5.x) in the stratosphere
  - mean differences are within ~5% down to tropopause height.
  - agreements of ~2-3% can be found for altitudes ~5 km above the tropopause.
  - SAGE III v5.2 MLR O3 retrieval is improved, which shows similar accuracy as AER retrieval in the UT/LS regions (v5.1 MLR ozone shows larger positive biases (>10%) below 20 km, compared to AER ozone).
  - The large sr/ss differences are reduced in v5.2 (and consistent with other satellite measurements), why?
  - MLS (v5.x) ozone profiles still show oscillation artifacts in the lower stratosphere, especially in the tropics.

- Larger sampling biases (5-10%) could be found in SAGE III monthly zonal mean ozone in high latitude stratosphere and in the UT/LS regions without correction.

- The 2-D regression model can be used to minimize sampling bias in derived climatologies (e.g. MZM) from SAGE III and other non-uniform satellite measurements.

Conclusions and future works

- Based on current studies, the sampling biases in SAGE III MZM can be reduced by 1-5% in the subtropical and midl-latitude UT/LS regions by applying corrections/adjustments.

- The 2-D regression model correction method does not work well in the tropical (20^oS-20^oN) and high latitude (60^0poleward) UT/LS regions. It could result from less measurements and not optimal regression model (predictors and/or number of Legendre polynomial and Fourier terms).

- Future studies:
  - To further investigate/improve sampling biases correction methods in regions that do not work well
  - Test the method by using other satellite data and/or model output
  - Apply final sampling bias correction method/algorithm to produce updated GOZCARDS ozone (H2O) dataset.

Thank you