SHADOZ (Southern Hemisphere Additional Ozonesondes): Data Archive and QA/QC Activities

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WMO ET-WDC Meeting, October 1-3, 2019

NASA Langley, Virginia, USA

Outline

- Scope of SHADOZ
  - Origins of SHADOZ: 14 stations, > 20 sponsoring organizations
  - Data Archive & Stations, > 8000 profiles
  - Data Flow & Meta-Data Handling
  - Reprocessed v6.0 SHADOZ data, released in March 2019
- SHADOZ Quality Assurance Activities, Science, and Validation Support
  - With WMO & NDACC: Quality Assurance & Capacity Building
  - Support to Satellite Community
  - SHADOZ Scientific Accomplishments

Origins of SHADOZ

- **SHADOZ Role:**
  - "Strategic" ozonesonde network that coordinates tropical launches for science.
  - Producer and provider of data and research archive for tropical and subtropical stations.
  - Support those who monitor O_3 trends for UNEP/WMO Assessments, Montreal Protocol.

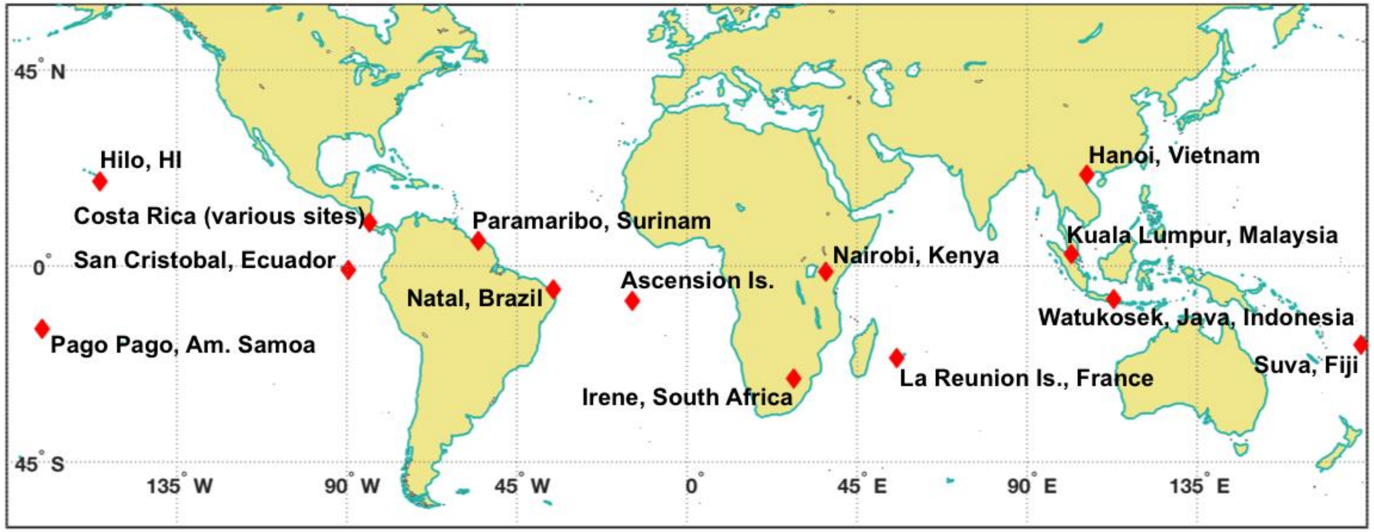
Milestones:

1998: 1 stable station, 8 intermittent stations

2009: NDACC & WMO/GAW affiliations

NOW: 14 sites with 10-yr record (right)

SHADOZ sites and partners

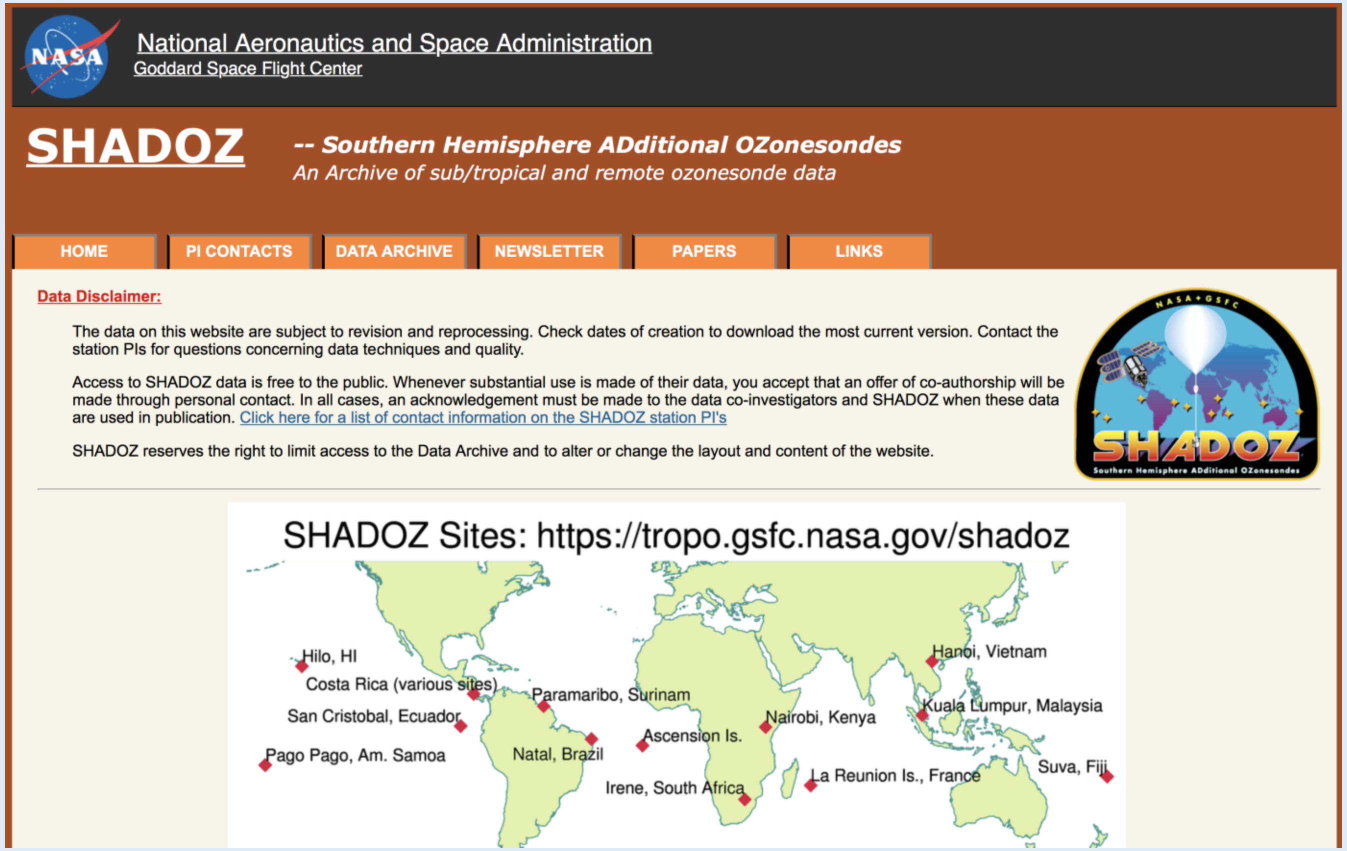


NOAA · NDACC · JAMSTEC · Ministério da Ciência e Tecnologia – Instituto Nacional de Pesquisas Espaciais · RISH – Research Institute for Sustainable Humanosphere, Kyoto University · Royal Netherlands Meteorological Institute · Hokkaido University · Université de La Réunion · USP – The University of the South Pacific · INAMHI · MET Malaysia · Kenya Meteorological Department · Universidad de Costa Rica · South African Weather Service · MeteoSwiss · NCAR

Data Archive & Stations List

- **Data Archive:** https://tropo.gsfc.nasa.gov/shadoz > 8000 O_3, PTU profiles, 1998-2019.
- We are a **research data archive** and not operational. Near-real time data transfer is not practical.

Station	Profile Total (Years)
Pago Pago, American Samoa	752 (1998-2019)
Hilo, Hawaii	1054 (1998-2019)
San Cristóbal, Galapagos, Ecuador	442 (1998-2008, 2012-2016)
San Pedro, Costa Rica	605 (2005-2019)
Paramaribo, Suriname	748 (1999-2018)
Ascension Island	710 (1998-2010, 2016-2019)
Natal, Brazil	653 (1998-2011, 2013-2018)
Irene, South Africa	374 (1998-2008, 2012-2019)
Nairobi, Kenya	905 (1998-2019)
La Réunion, France	647 (1998-2018)
Kuala Lumpur, Malaysia	427 (1998-2010, 2012-2018)
Hanoi, Vietnam	268 (2004-2018)
Watukosek, Java, Indonesia	343 (1998-2013)
Suva, Fiji	437 (1998-2019)



Data Flow and Meta-Data Handling

- Collect data (including meta-data) where station operators use standard form (**right**) to record meta-data to facilitate data reprocessing.
- **Data Flow:** Station operator -> Sponsor/Co-I -> SHADOZ data archiver -> Data Reprocessing -> SHADOZ website
- ***Required metadata fields*** are those variables that appear in the Electrochemical Concentration Cell (ECC) ozonesonde equation and describe the conversion from the measured raw cell current to ozone partial pressure.

$$P_{O_3} = \frac{R}{2F} \cdot \gamma(P) \cdot \frac{t_{100}}{\eta_{t_{100}}} \cdot \mathrm{T_{pump}} \cdot (\mathrm{I} - I_{bg}) \qquad (1)$$

where:

- R = Ideal gas constant
- F = Faraday constant
- $\gamma(P)$ = Pressure dependent pump efficiency correction factor []
- P = Air pressure
- t_{100} = Time to pump 100 ml of laboratory air $[\frac{s}{100\ ml}]$
- η_{t100} = Humidity correction for flow rate []
- I_{bg} = Background current [μA]
- T_{pump} = Measured pump temperature [K]
- I = Measured cell current [μA]

Version: Mar 26, 2018 **SHADOZ DIGITAL OZONESONDE CHECKLIST**

INITIAL PREPARATION - NO LESS THAN 3 DAYS BEFORE FLIGHT. **Operator Initials:**_______

DATE (YYYYMMDD): ___________________ **ECC SONDE SERIAL #:** ___________________
STATION ___________________ **Sensing Solution/Buffer:** ___________________
Cathode Volume: 3.0cc ____ **or** 2.5cc ____ (√)

1. Run 10 minutes on *no* O_3 air: ____ (√)
2. Pump Current: __________ (units?)
3. Pump Pressure: __________ (units?)
4. Pump Vacuum: __________ (units?)
5. Bypass Cathode chamber: Yes ___ No ___
6. IF YES Add 5.5cc Cathode solution: ____ (√)
7. Run 30 minutes on *HIGH* O_3: ____ (√)
8. Run 5 minutes on *no* O_3: ____ (√)
9. Dump Cathode solution IF Cathode cell bypassed: ____ (√)
10. Add the Cathode solution (Wait 2-5 min): ____ (√)
11. Add 1.5 CC Anode solution: ____ (√)
12. Run 10 minutes on *no* O_3: ____ (√)
13. Record O_3 Current: ________ μA
14. Run 10 minutes at 5μA O_3 ____ (√)
15. Switch to *no* O_3 air ____ (√)
16. Record time to drop from 4 to 1.5 μA: _______ sec.
17. Run 10 minutes on *no* O_3: ____ (√)
18. Record O_3 Current: ________μA
19. Add additional 2.5 cc of Cathode ONLY: Yes ___ No ___
20. Short the cell leads: ____ (√)
21. Store in sonde box: ____ (√)
22. Rinse syringes: ____ (√)

IF DORMANT AFTER 1 WEEK REPLACE SOLUTIONS. **DATE (YYYYMMDD) :** _________________

1. Change Cathode Solution (3cc or 2.5cc): ____ (√)
2. Change Anode Solution (1.5cc): ____ (√)
3. Run 5 minutes on *no* O_3 ____ (√)
4. Record O_3 Current: ________ μA
5. Run 5 minutes on 5μA O_3 ____ (√)
6. Switch to *no* O_3: ____ (√)
7. Time to drop from 4 to 1.5μA: ________ sec
8. Run 10 minutes on *no* O_3 then Record Current: _________ μA
9. Add additional 2.5 cc of Cathode ONLY: Yes ___ No ___
10. Short cell leads, store in sonde box, rinse syringes: ____ (√)

DAY OF FLIGHT PREPARATION: DATE (YYYYMMDD): ________________ INITIALS: _____

1. Cathode solution # and date of bottle *(if applicable)*: ____________________________
2. Remove original Cathode and Anode solution ____ (√)
3. Rinse cells by adding Cathode and Anode and removing ____ (√)
4. Add Cathode solution (wait 2-5 min): ____(√)
5. Add Anode solution: ____ (√)
6. Run 10 minutes on *no* O_3: ____ (√)
7. Record O_3 Current: IB0 = _________ μA
8. Run 10 minutes at 5μA O_3: ____ (√)
9. Switch to *no* O_3: ____ (√)
10. Record time to drop from 4 to 1.5 μA: _________ sec
11. Run 10 minutes on *no* O_3 then record O_3 Current: IB1 = __________ μA
12. **Room T(C)** _______, **RH(%)**______, **P(hPa)** _______
13. RECORD 5 FLOWRATES (sec/100ml):
    #1: __________, #2: __________, #3: __________
    #4: __________, #5: __________, AVERAGE:________
14. Flowrate Correction *(if applied)*________(%)
15. **Final Flowrate**:_________

DAY OF FLIGHT LAUNCH PREPARATION **FLT #:** __________ INITIALS: ______

RADIOSONDE TYPE/Model (e.g. Vaisala RS92, Modem M10, etc): ____________________
RADIOSONDE SERIAL #: _________________ INTERFACE # *(if known)*:____________________
O_3 Background current used before launch: IB2 = __________ μA, **Final IB used**: __________ μA
GMT Launch Date (YYYYMMDD): _________________
GMT Launch Time (HH:MM:SS): ______________ ***LOCAL*** Launch Time (HH:MM:SS): ______________

BALLOON SIZE: ___________Grams: TYPE: Totex ____ Hwoyee ____ PAWAN ____ (√ one)
NOAA FPH ____ (√) or CFH ____ (√) Serial # *(if applicable)*: ____________________
Surface Pressure: ______________(hPa) Surface Wind Speed: __________ (m/s)
Surface Temp: ______________ (C) Surface Wind Direction: ___________ (deg)
Surface RH: ________________ (%) Sky Conditions and Remarks: ________________________

DOBSON ____ **(√), BREWER** ____ **(√), Other (√)** ____________: ____________**(DU)**

Reprocessed v6.0 SHADOZ Data References

- Series of Assessment of Standard Operating Procedures for Ozonesondes (ASOPOS) meetings led to WMO Report 201 on ozonesonde procedures.
- Reprocessing approach based on ASOPOS guidelines. Update to these guidelines forthcoming in 2020.

- **Reprocessing:**
  1. SHADOZ Reprocessing: Witte et al., JGR, doi:10.1002/2016JD026403 [2017]
  2. NOAA Reprocessing: Sterling et al., AMT, doi:10.5194/amt-2017-397 [2018]
  3. WFF Reprocessing: Witte et al., JGR, doi:10.1029/2018JD030098 [2019]
- **Evaluation:**
  1. Thompson et al., JGR, doi:10.1002/2017jd027406 [2017]
  2. JOSIE-SHADOZ Experience: Thompson et al., BAMS, doi:10.1175/BAMS-D-17-0311.1 [2018]
- **Uncertainties**: Witte et al., JGR, doi:10.1002/2017JD027791 [2018]

AGU PUBLICATIONS

JGR

Journal of Geophysical Research: Atmospheres

RESEARCH ARTICLE
10.1002/2016JD026403

Key Points:
- This is the first major reprocessing of SHADOZ ozonesonde data records
- The effect of reprocessing is observed throughout the profile, and the magnitude of change is highly variable and station dependent
- Reductions in satellite biases are due to ozonesonde reprocessing techniques that correct for errors in operating procedures

Supporting Information:
- Table S1

First reprocessing of Southern Hemisphere ADditional OZonesondes (SHADOZ) profile records (1998–2015): 1. Methodology and evaluation

Jacquelyn C. Witte[1,2], Anne M. Thompson[2], Herman G. J. Smit[3], Masatomo Fujiwara[4], Françoise Posny[5], Gert J. R. Coetzee[6], Edward T. Northam[1,7], Bryan J. Johnson[8], Chance W. Sterling[8,9], Maznorizan Mohamad[10], Shin-Ya Ogino[11], Allen Jordan[8,9], and Francisco R. da Silva[12]

[1]Science Systems and Applications Inc., Lanham, Maryland, USA, [2]NASA/Goddard Space Flight Center, Greenbelt, Maryland, USA, [3]Institute of Chemistry and Dynamics of the Geosphere: Troposphere, Research Centre Juelich, Juelich, Germany, [4]Faculty of Environmental Earth Science, Hokkaido University, Sapporo, Japan, [5]Department of Physics, University of La Réunion Island, Réunion, France, [6]South African Weather Service, Erasmusrand, Pretoria, South Africa, [7]NASA/Wallops Flight Facility, Wallops Island, Virginia, USA, [8]Global Monitoring Division, NOAA, Earth System Research Laboratory, Boulder, Colorado, USA, [9]Cooperative Institute for Research in Environmental Sciences, University of Colorado Boulder, Boulder, Colorado, USA,

AGU PUBLICATIONS

JGR

Journal of Geophysical Research: Atmospheres

RESEARCH ARTICLE
10.1002/2017JD027791

Key Points:
- First estimates of ECC ozonesonde uncertainties using SHADOZ data records
- Ozone uncertainties are generally within 15% and peak around the tropopause where ozone measurements approach the uncertainty estimates
- Uncertainties in background and sensor current dominate the troposphere, while conversion efficiency and flow rate dominate the stratosphere

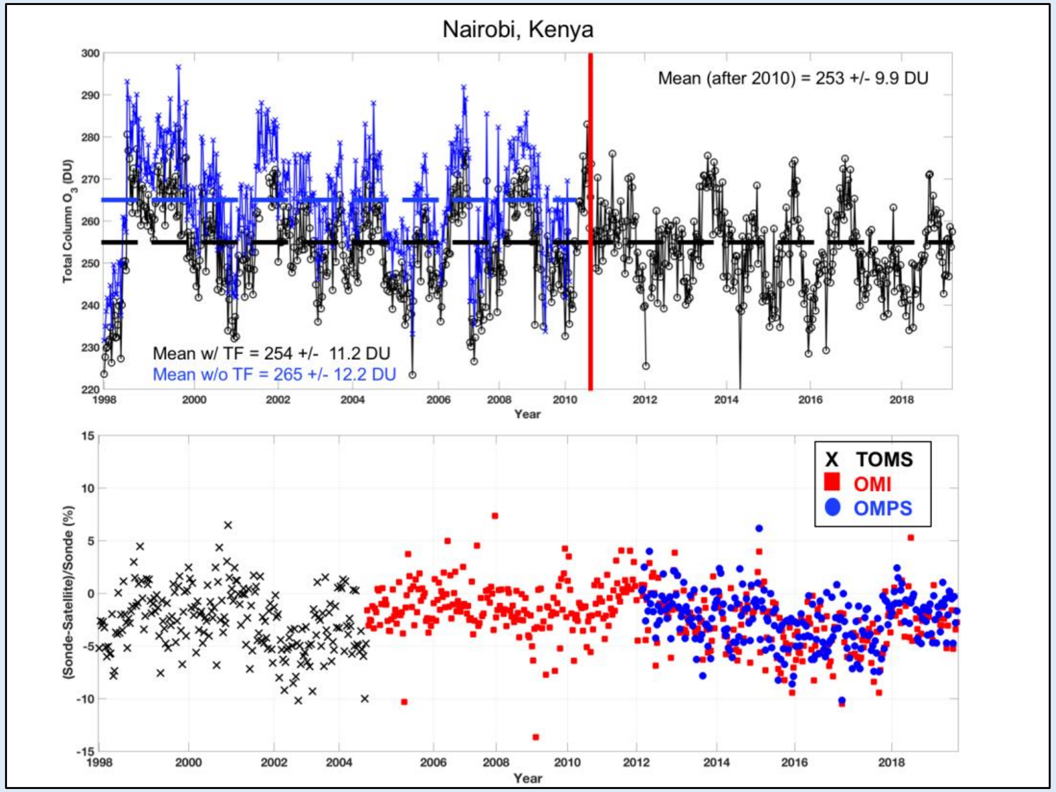
First Reprocessing of Southern Hemisphere ADditional OZonesondes Profile Records: 3. Uncertainty in Ozone Profile and Total Column

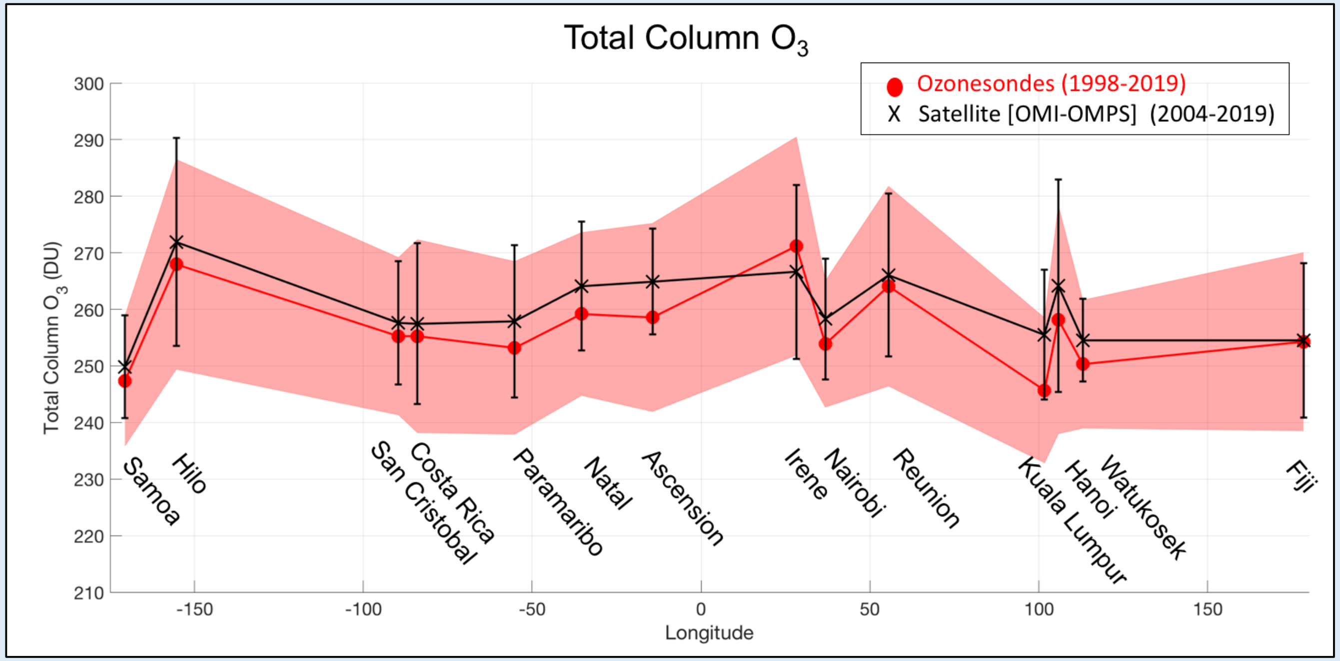
Jacquelyn C. Witte[1,2], Anne M. Thompson[2], Herman G. J. Smit[3], Holger Vömel[4], Françoise Posny[5], and Rene Stübi[6]

[1]Science Systems and Applications, Inc., Lanham, MD, USA, [2]NASA Goddard Space Flight Center, Greenbelt, MD, USA, [3]Institute of Chemistry and Dynamics of the Geosphere: Troposphere, Research Centre Jülich, Jülich, Germany, [4]Earth Observing Laboratory, National Center for Atmospheric Research, Boulder, CO, USA, [5]Laboratoire de l'Atmosphère et des Cyclones, UMR8105, Université, Météo-France, CNRS, La Réunion, France, [6]Federal Office of Meteorology and Climatology MeteoSwiss, Payerne, Switzerland

Reprocessed v6.0 SHADOZ Data Examples

- **Example of Data Reprocessing for Nairobi station (bottom left):**
  - A transfer function (TF) based on Deshler et al. (2017) is applied to the Nairobi 1998 to October 2010 data to convert O_3 measured with a nonstandard ENSCI ECC/1% full buffer sensing solution type (SST) to WMO and manufacturer recommended ENSCI/0.5% half buffer equivalent.
  - ~11 DU difference in Total Column Ozone (TCO) before and after reprocessing data.
- **TCO Comparisons with Satellites (bottom right):** All stations agree 5% or better.





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Partnerships and Capacity Building

KNMI, GSFC & MDS: Paramaribo

MeteoSwiss: Nairobi, Kenya

NOAA: Fiji (L), Ecuador (R)

NOAA: Hilo, HI

GSFC & USAF: Ascension Island, U.K.

JAMSTEC: Hanoi, Vietnam

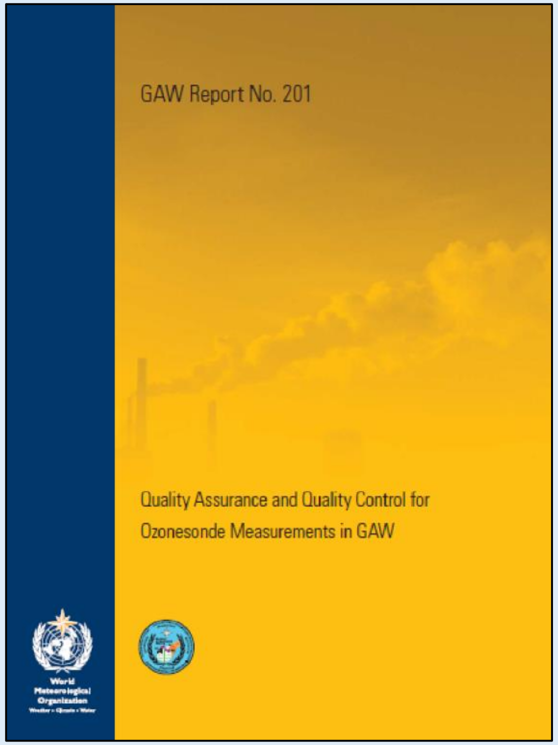
GSFC & NCAR: San Pedro, Costa Rica

Recent SHADOZ QA/QC Activities

(L): JOSIE-SHADOZ 2017 Participants
(R): Station operators during JOSIE-SHADOZ 2017

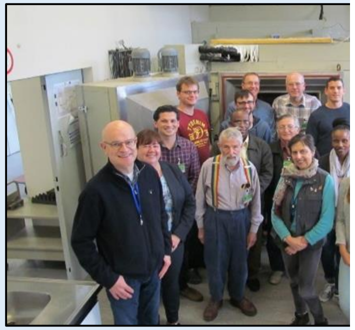
The World Calibration Center for Ozonesondes (WCCOS)

Date	Activity
2011-2014	ASOPOS Panel (WMO/GAW no. 201) →
2011-2015	WCRP SPARC SI^2N
Aug. 2012	QOS Toronto
2015-2016	**Major SHADOZ Reprocessing (v6 data)**
Sep. 2016	QOS Edinburgh
Sep.-Oct. 2017	JOSIE-SHADOZ 2017
Sep. 2018	ASOPOS 2.0 Panel Meeting in Geneva
Sep. 2019	ASOPOS 2.0 Panel Meeting in Brussels
End of 2020	New WMO/GAW Report Delivered



WMO/GAW Report no. 201

Recent SHADOZ QA/QC Activities



(L): JOSIE-SHADO
(R): Station opera

The World Calibra

JOSIE-SHADOZ 2017 in the Bulletin of the American Meteorological Society (BAMS), January 2019:

OZONESONDE QUALITY ASSURANCE

The JOSIE–SHADOZ (2017) Experience

Anne M. Thompson, Herman G. J. Smit, Jacquelyn C. Witte, Ryan M. Stauffer, Bryan J. Johnson, Gary Morris, Peter von der Gathen, Roeland Van Malderen, Jonathan Davies, Ankie Piters, Marc Allaart, Françoise Posny, Rigel Kivi, Patrick Cullis, Nguyen Thi Hoang Anh, Ernesto Corrales, Tshidi Machinini, Francisco R. da Silva, George Paiman, Kennedy Thiong'o, Zamuna Zainal, George B. Brothers, Katherine R. Wolff, Tatsumi Nakano, Rene Stübi, Gonzague Romanens, Gert J. R. Coetzee, Jorge A. Diaz, Sukarni Mitro, Maznorizan Mohamad, and Shin-Ya Ogino

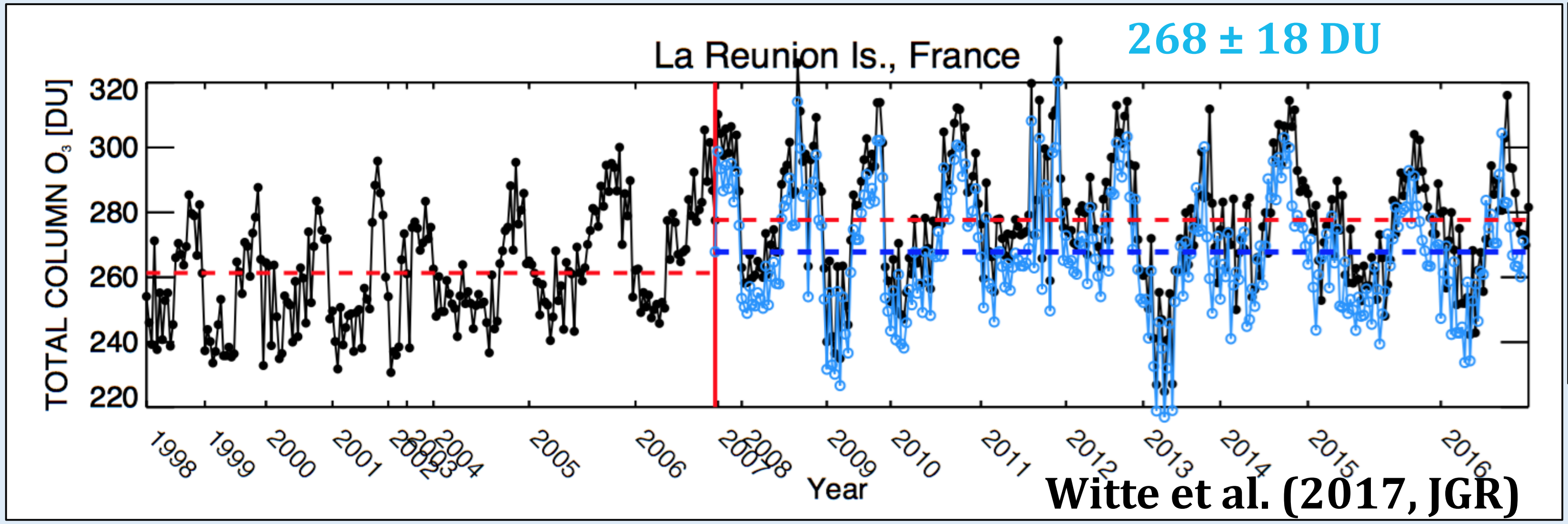
As a backbone for satellite algorithms and monitoring stratospheric ozone recovery, ozonesondes require regular evaluation, here performed by operators of the tropical SHADOZ network.

Thompson et al. (2019, BAMS)

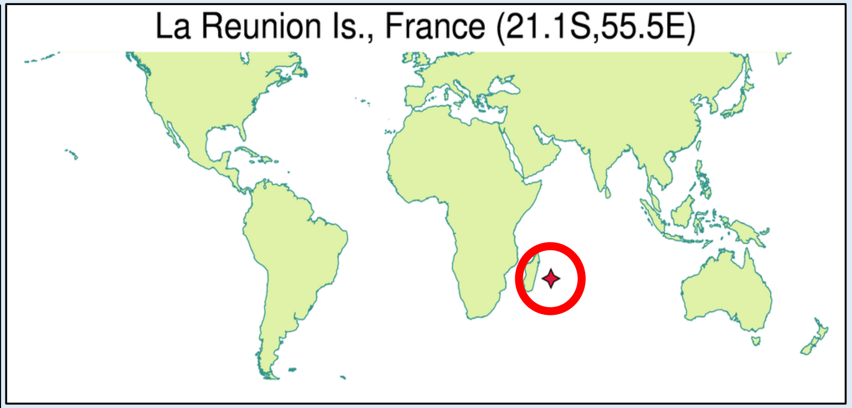
W Report no. 201

QA/QC Activities Lead to Reprocessing

261 ± 17 DU **278 ± 19 DU** **268 ± 18 DU**



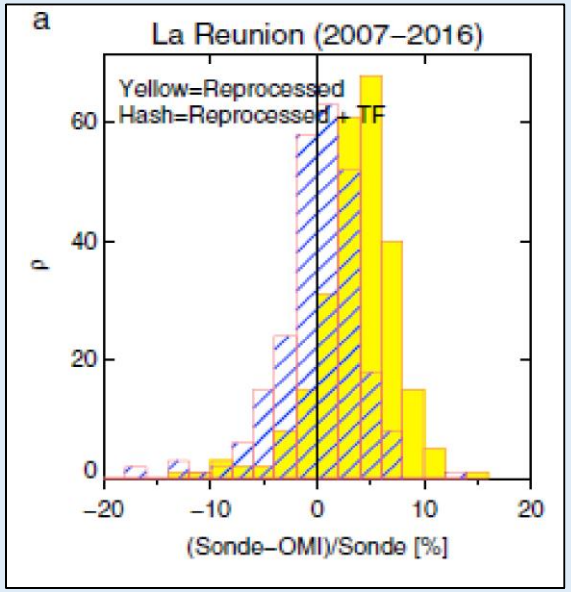
Witte et al. (2017, JGR)

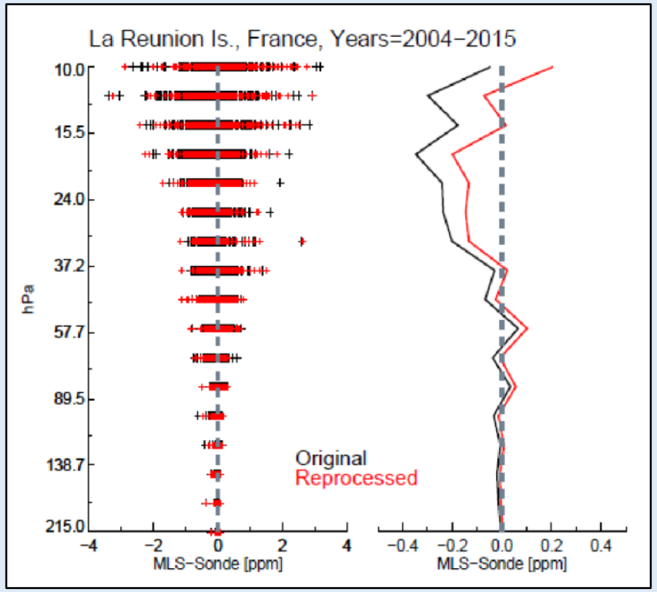


Upper: Discontinuity disappears after homogenization (applied transfer function) (blue line -> v6 data).

Left: Total ozone with correction (hashed) agrees better with OMI.

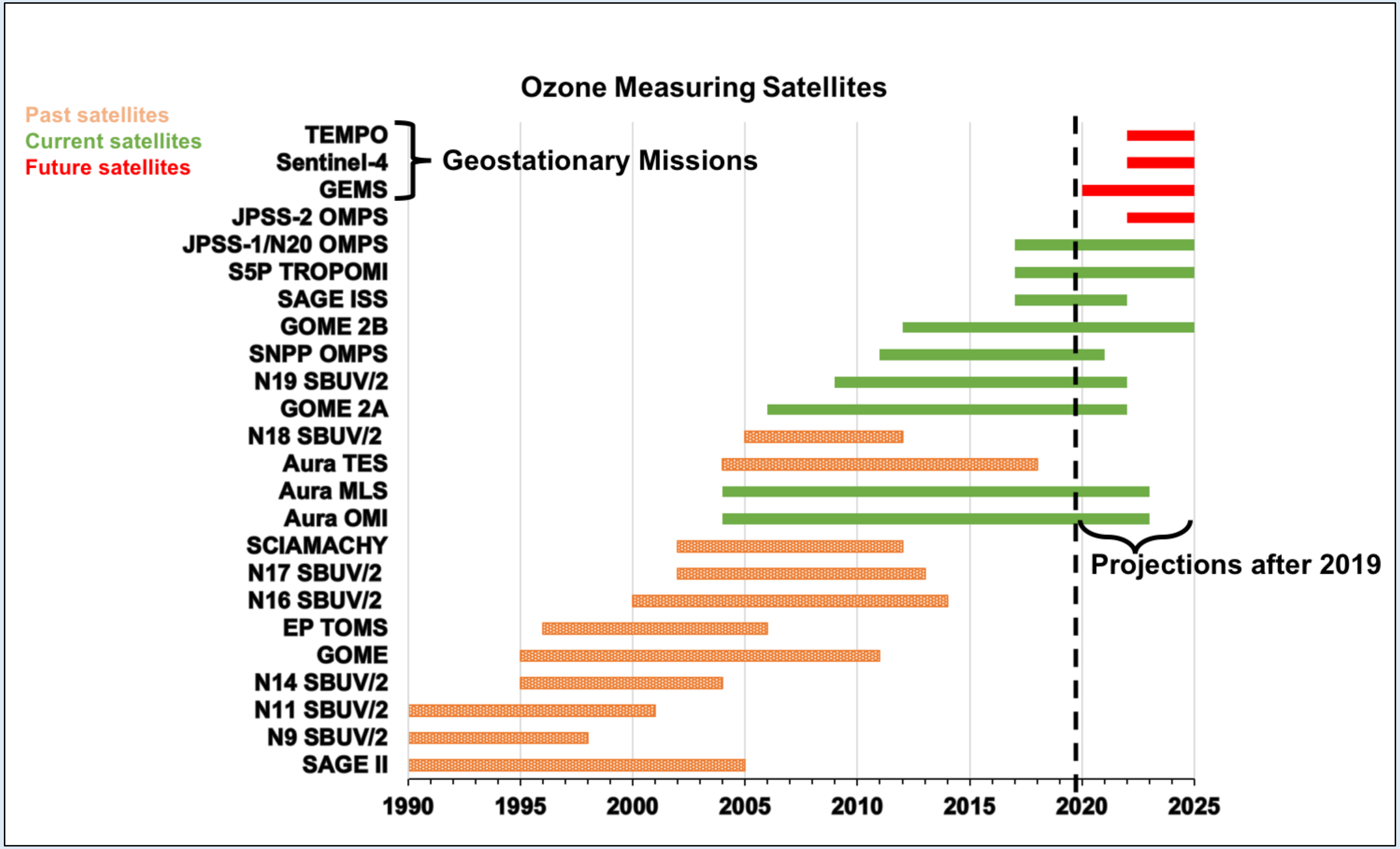
Right: Most post-processing improvement is in the stratosphere. Sondes now closer to Aura/MLS O_3 profile (red).





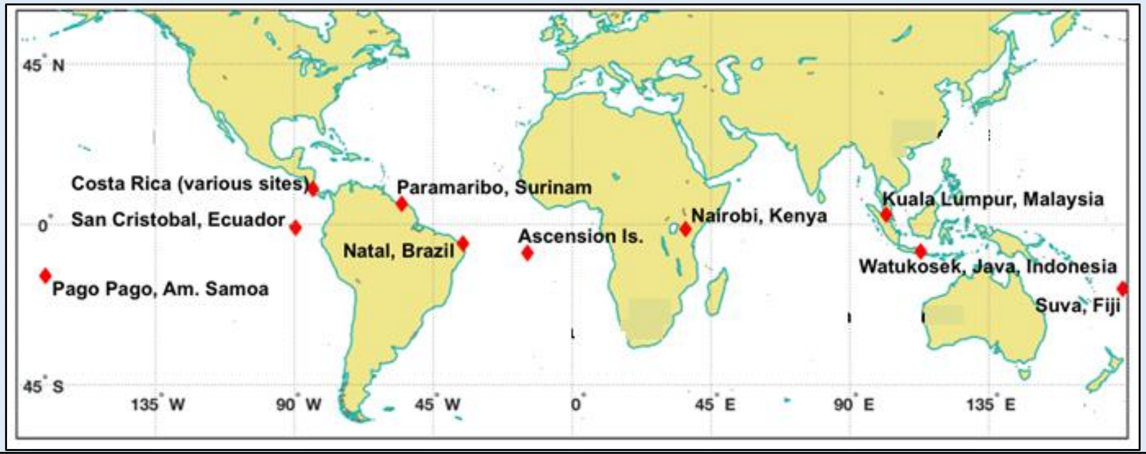
SHADOZ Validates Satellite Missions

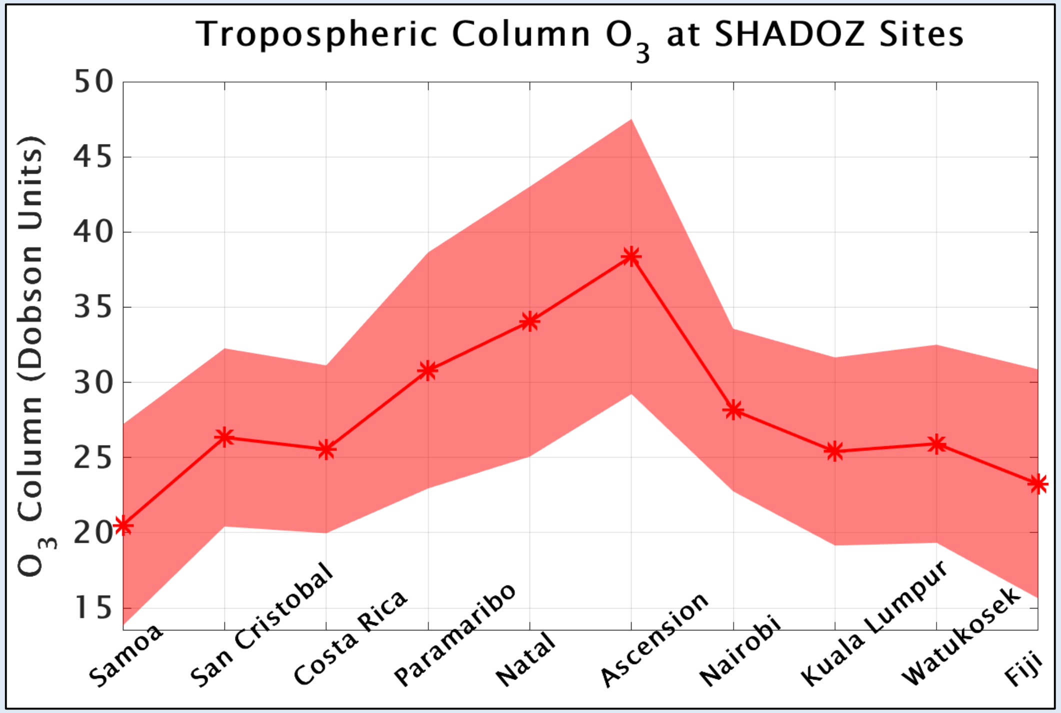
- The SHADOZ Archive has supported dozens of satellite missions
- A major goal of reprocessing is to provide stable, long-term records of ozonesonde data for satellite cal/val and trend comparisons (goal of 5% uncertainty)

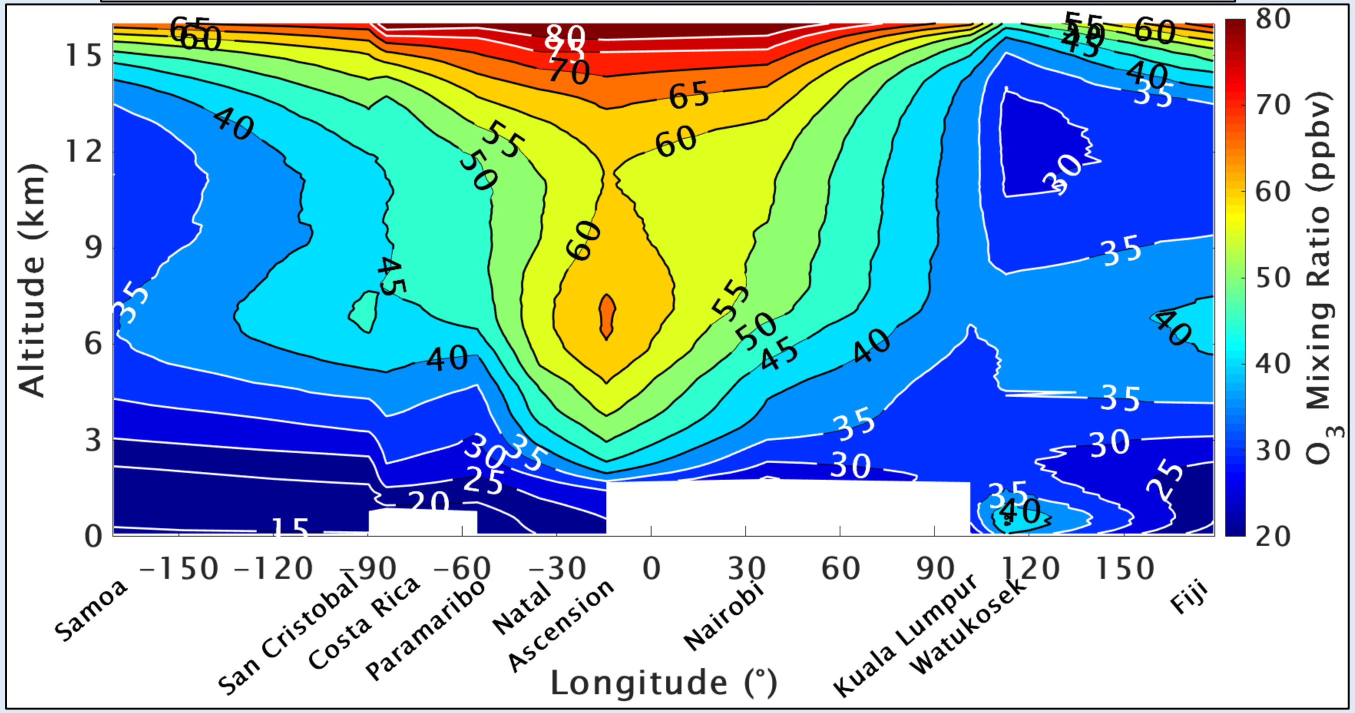


SHADOZ Scientific Accomplishments

- A tropical "wave-one" pattern in total ozone was first identified by satellite measurements in 1980s
- SHADOZ data revealed that this feature resides entirely in the troposphere
- This information now aids satellite ozone retrieval algorithm development



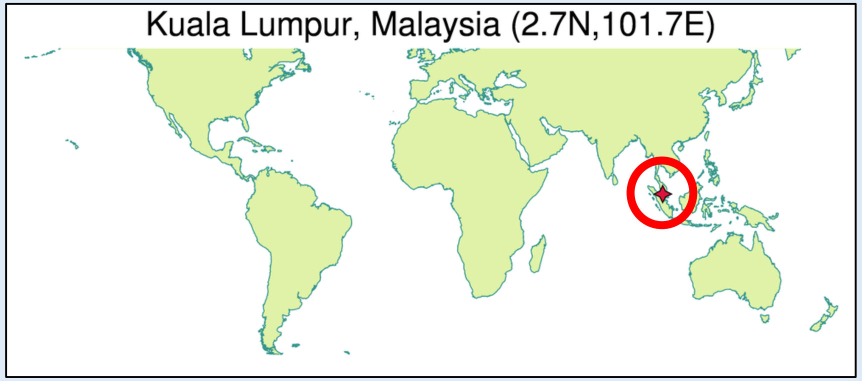


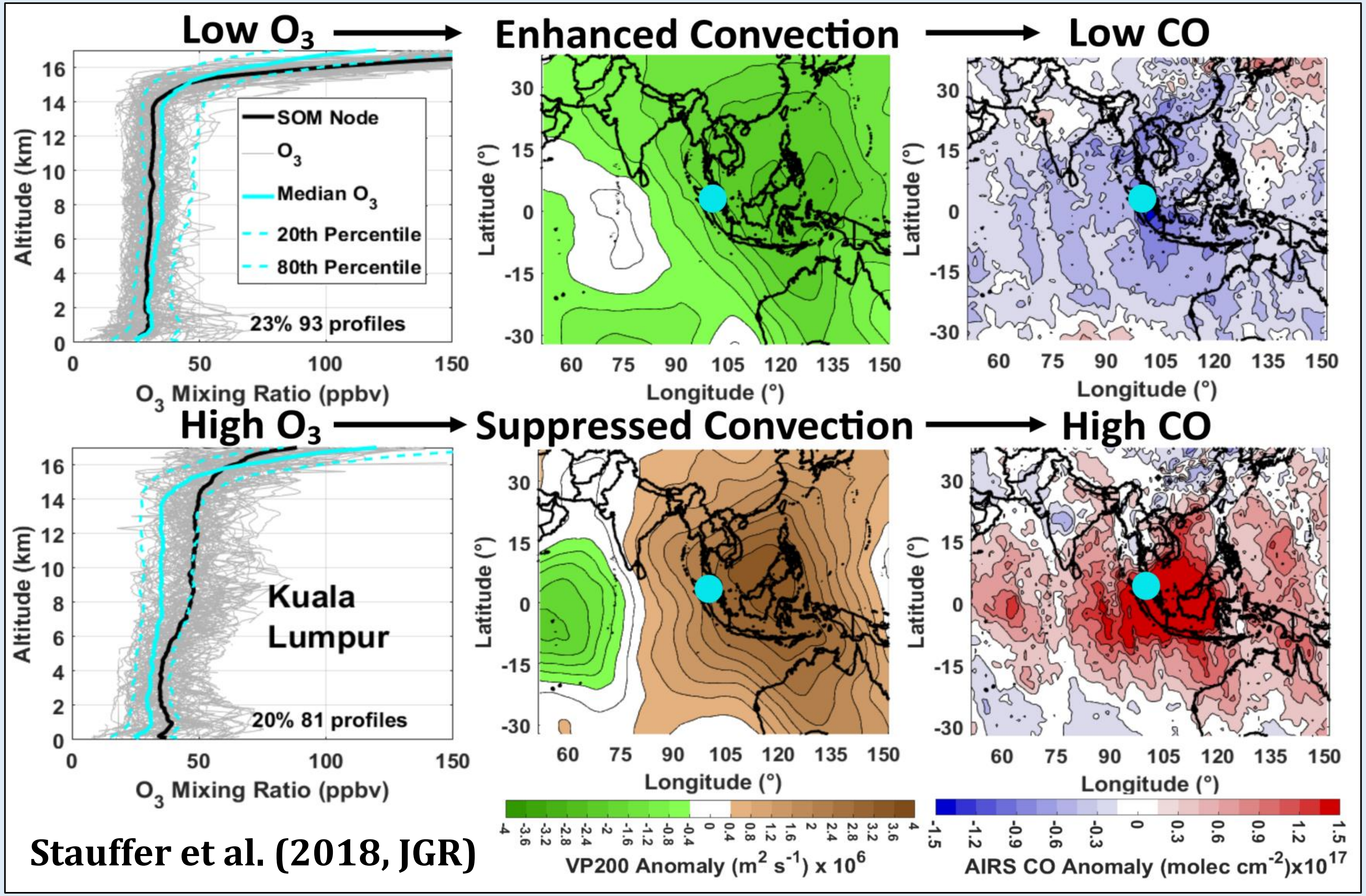


SHADOZ Scientific Accomplishments

- With 20+ years of reprocessed data, we can form meaningful ozone climatologies and perform robust statistical analyses

- Example from Kuala Lumpur, Malaysia, shows the relationship between ozone amount (**L**), convection (**C**), and carbon monoxide pollution (**R**)





Stauffer et al. (2018, JGR)

Thank You to Sponsors, Partners and Collaborators!

Major Partners: NOAA/GMD, NASA Wallops

NASA HQ: M. Kurylo (1998-2008), K. Jucks (2008->) and J. Kaye

SHADOZ – 20 Years in 2018! Partners in US Europe, Asia & Africa, with visible data & engaged in WMO/NDACC O_3 "Community," maintain operations

THANK YOU, DATA USER COMMUNITY