

# Exploring SO<sub>2</sub> Profiling Capabilities Using Pandora MAX-DOAS Measurements

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Environment and  
Climate Change Canada



UNIVERSITY OF  
TORONTO

# Motivation: SO<sub>2</sub> Profiling

Sulfur Dioxide  
(SO<sub>2</sub>)

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graph TD; A[Sulfur Dioxide (SO2)] --> B[Natural sources: volcanic emissions (active & passive), biological decay]; A --> C[Anthropogenic sources: fossil fuel combustion and smelting of sulfur-containing mineral ores];
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Natural sources: volcanic emissions (active & passive), biological decay

Anthropogenic sources: fossil fuel combustion and smelting of sulfur-containing mineral ores

# Motivation: SO<sub>2</sub> Profiling

SO<sub>2</sub> lifetime: ~ few days  
Sulfate aerosol lifetime: ~ weeks



SO<sub>2</sub> lifetime: ~ several weeks  
Sulfate aerosol lifetime: ~ years

## Tropospheric Impacts:

- It is an atmospheric pollutant with direct & indirect human respiratory health implications
- It can be oxidized to form sulfate aerosols which impact the radiative budget and therefore climate
- It can produce acid rain as H<sub>2</sub>SO<sub>4</sub>

## Stratospheric Impacts:

- It is a significant source of stratospheric aerosols → stratospheric warming and tropospheric cooling
- Can partake in sulfidation reactions in airplane engines, which impacts aviation safety
- Can partake in stratospheric ozone depletion

# Motivation: SO<sub>2</sub> Profiling

- Early 1980s: Total Ozone Mapping Spectrometer (TOMS) detected volcanic sources
- 1995: Global Ozone Monitoring Experiment (GOME) detected anthropogenic sources
- 2000s-2010s: Ozone Monitoring Instrument (OMI), SCanning Imaging Absorption spectroMeter for Atmospheric CHartography (SCIAMACHY), Global Ozone Monitoring Experiment-2 (GOME-2), Ozone Mapping and Profiler Suite (OMPS) monitored regional and global SO<sub>2</sub> as well as point source emissions
- 2017: TROPOspheric Monitoring Instrument (TROPOMI) measures SO<sub>2</sub> with unprecedented spatial resolution, 3.5 km by 7 km (3.5 km by 5.5 km since 6 August 2019)

# Motivation: SO<sub>2</sub> Profiling

## Importance of retrieving SO<sub>2</sub> Profiles:

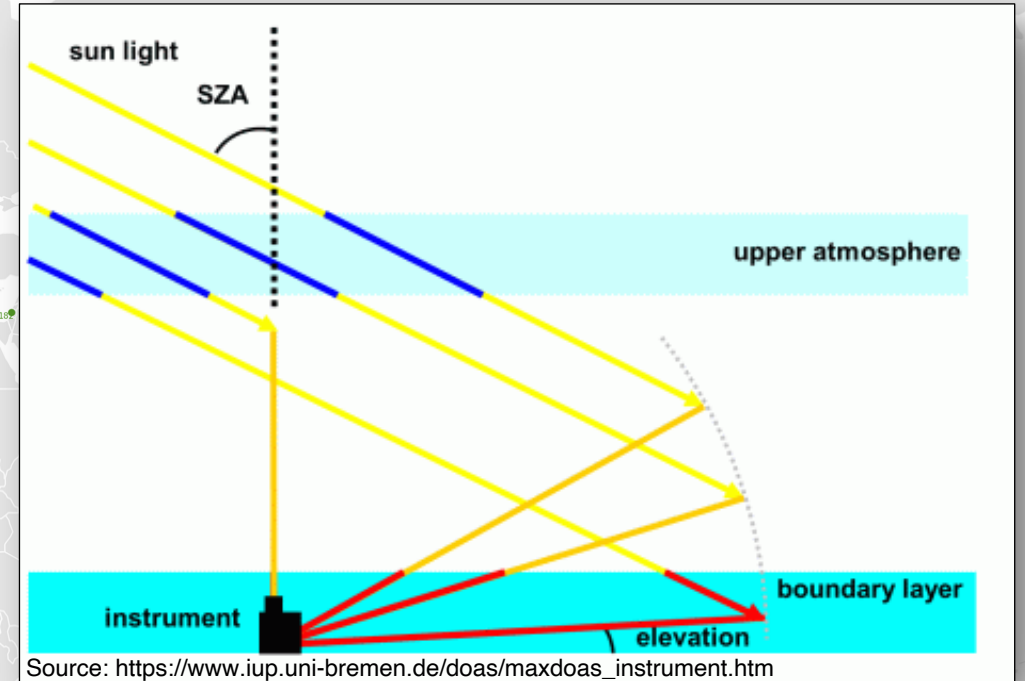
- (1) Important consideration for aviation (recall sulfidation reactions in engines)
- (2) Significance to atmospheric chemistry and climate (e.g., how will volcanic eruptions affect climate forcing?)
- (3) Estimation of SO<sub>2</sub> emissions (need vertical distribution of SO<sub>2</sub> for emission estimate)
- (4) Important consideration for human health exposure
- (5) Ground-based validation opportunities for satellite measurements of SO<sub>2</sub> plume heights, such as the TROPOMI COBRA SO<sub>2</sub> Layer Height (Theys et al., 2022)

# Methods: Pandora MAX-DOAS

P144 at Eureka-PEARL



P101 at Izana



PGN status

official non official

real time ● ●

delayed

# Volcanic Plumes at Pandora Sites

## Pandora I01 at Izana

Cumbre Vieja erupted from September 19 – December 2021

- Emitted 0.5 Tg of SO<sub>2</sub> to the atmosphere
- Estimated plume heights of 3-5 km, indicating no stratospheric injection
- Izana located ~140 km away from volcano

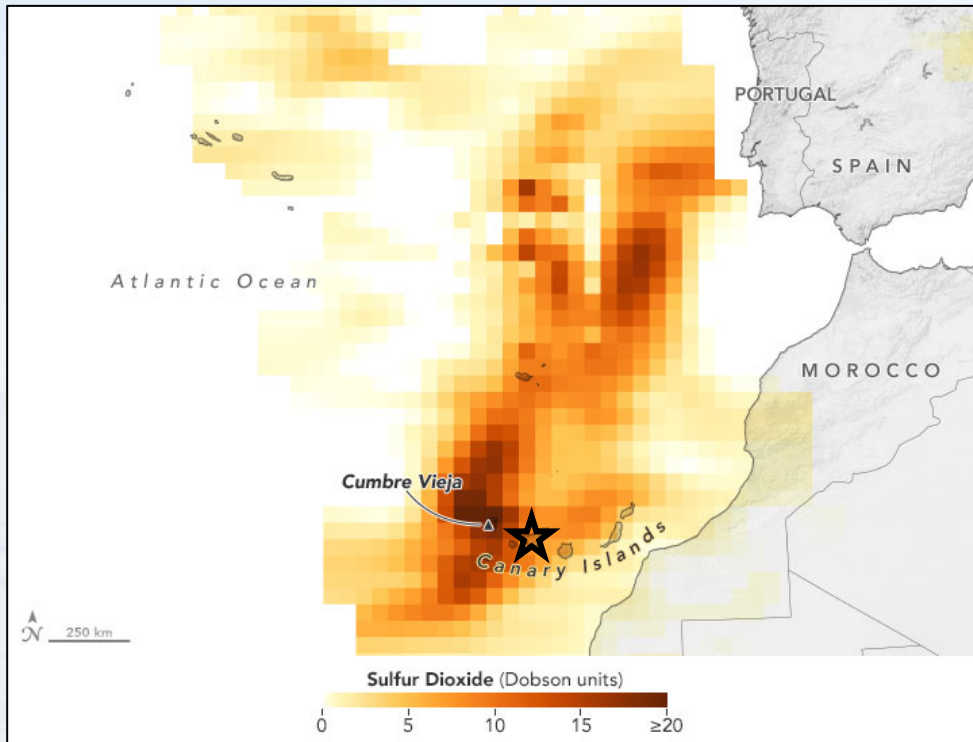
## Pandora I44 at Eureka-PEARL

Raikoke erupted on June 21–22, 2019

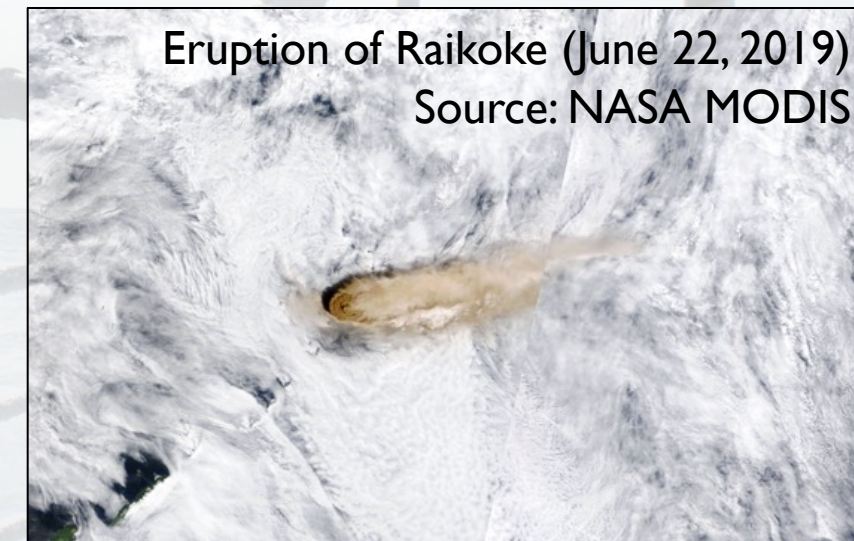
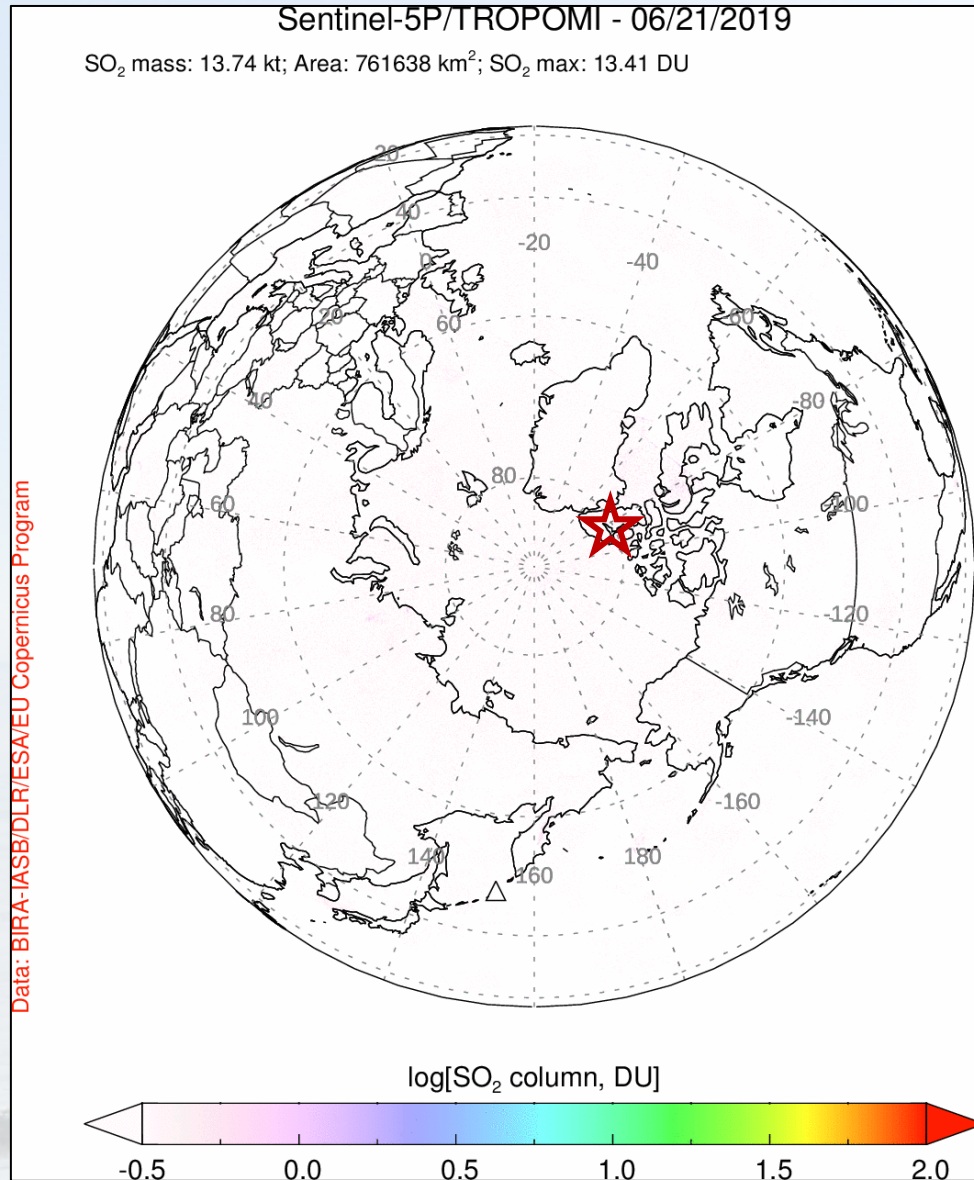
- Emitted 1.5 Tg of SO<sub>2</sub> to the atmosphere
- Estimated plume heights of 13 km, indicating stratospheric injection
- Reached Eureka, Nunavut on 4 July 2019

**Objective:** using Cumbre Vieja and Raikoke as case studies, enable SO<sub>2</sub> profiling and downwind plume height determination from ground-based Pandora instruments

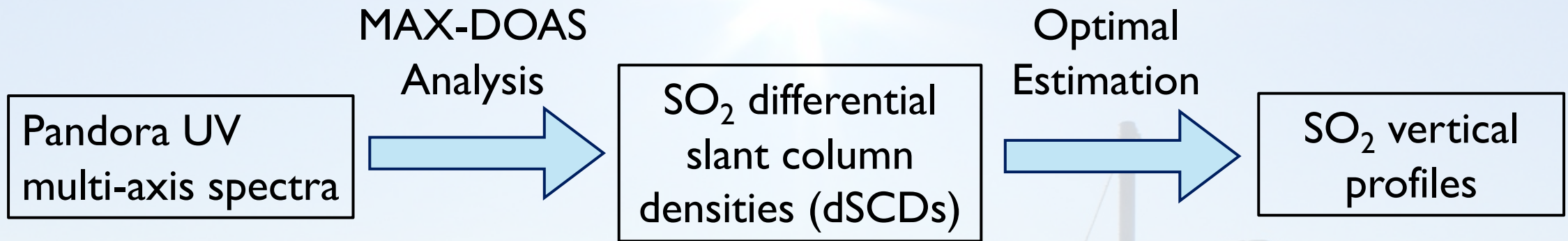
# Case Study I: Cumbre Vieja Plume at Izana



# Case Study 2: Raikoke Plume at Eureka-PEARL



# Methods: Pandora SO<sub>2</sub> Profiling



## Questions:

- Can Pandora multi-axis data be used to successfully derive plume heights from volcanic eruptions?
- What is the spatiotemporal distribution of the SO<sub>2</sub> plume heights downwind?
- Can this method be successfully used for other events with high SO<sub>2</sub> conditions, such as near power plants, oil refineries, etc.?

# Methods: Pandora MAX-DOAS

Pandora UV  
multi-axis spectra

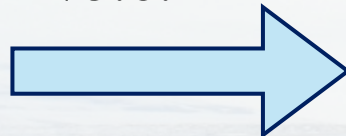
MAX-DOAS

Analysis

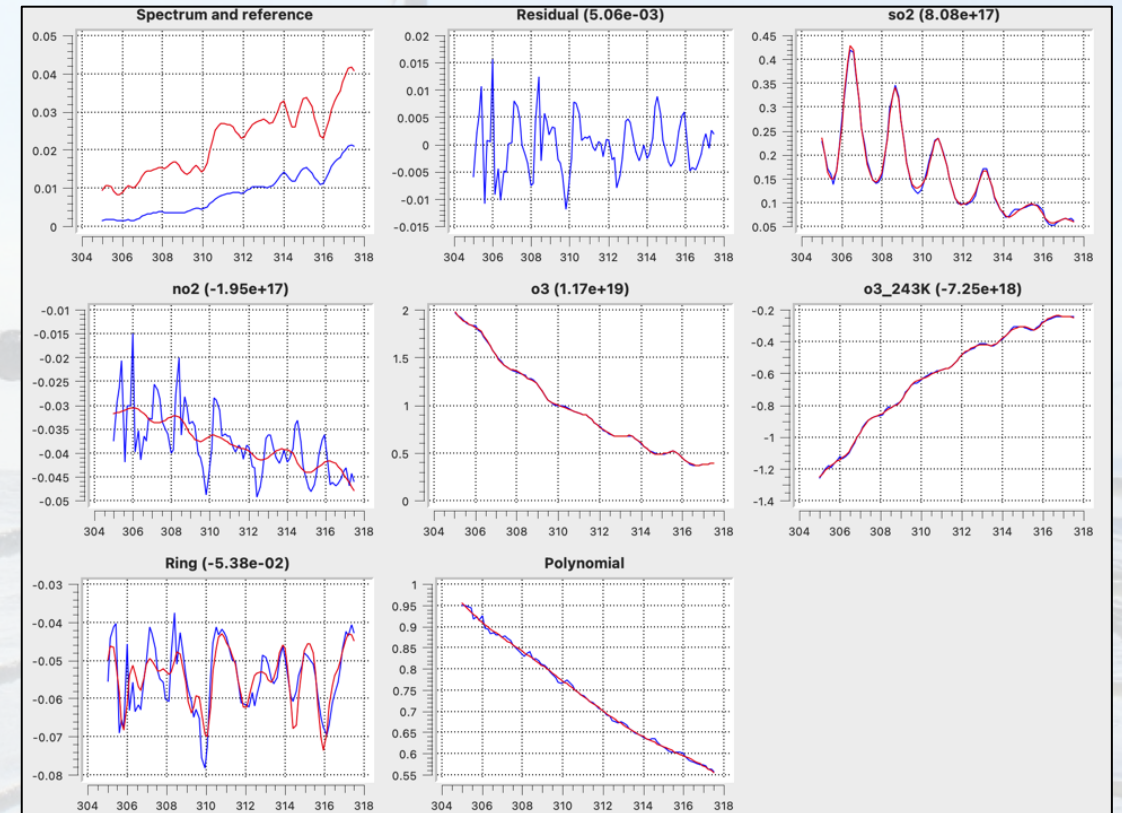
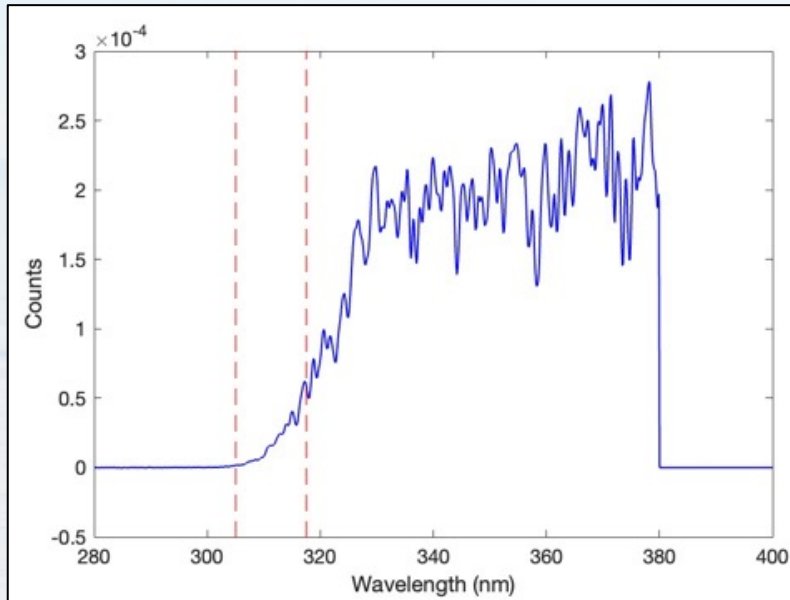


SO<sub>2</sub> dSCDs

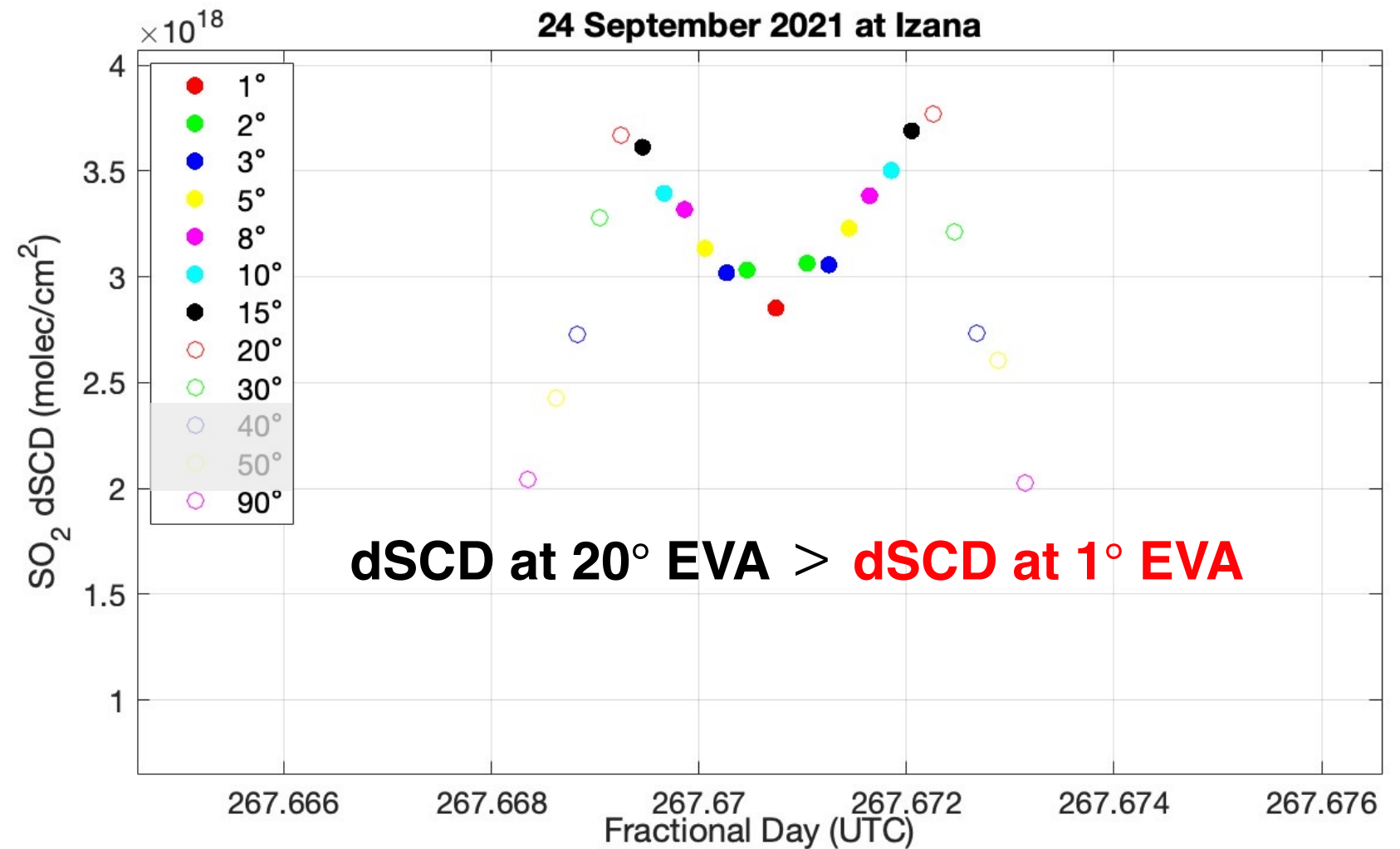
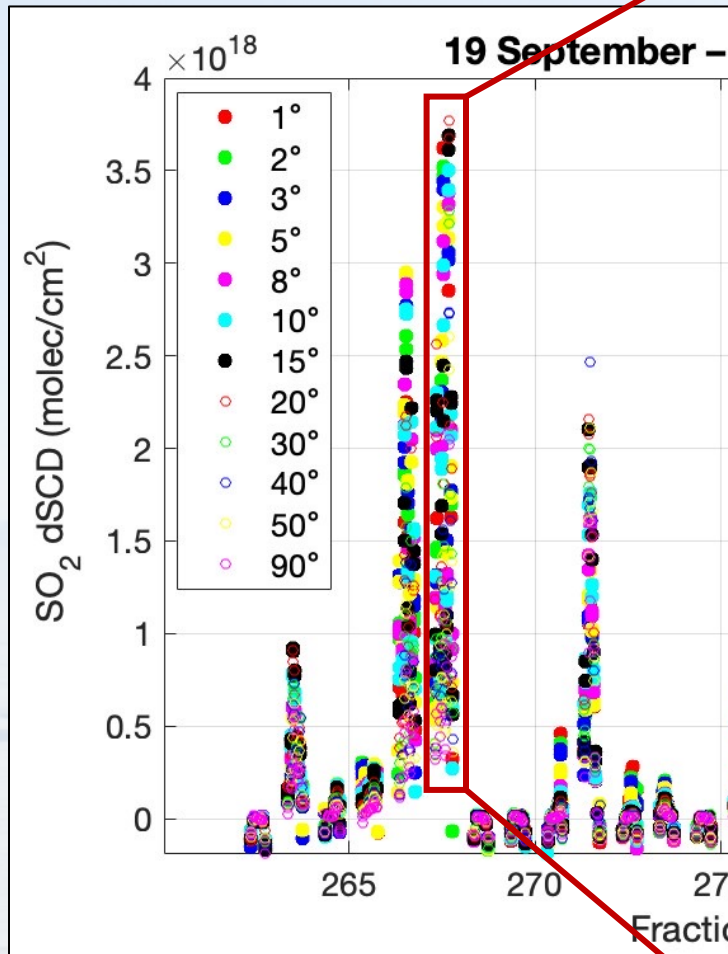
QDOAS  
v3.6.11



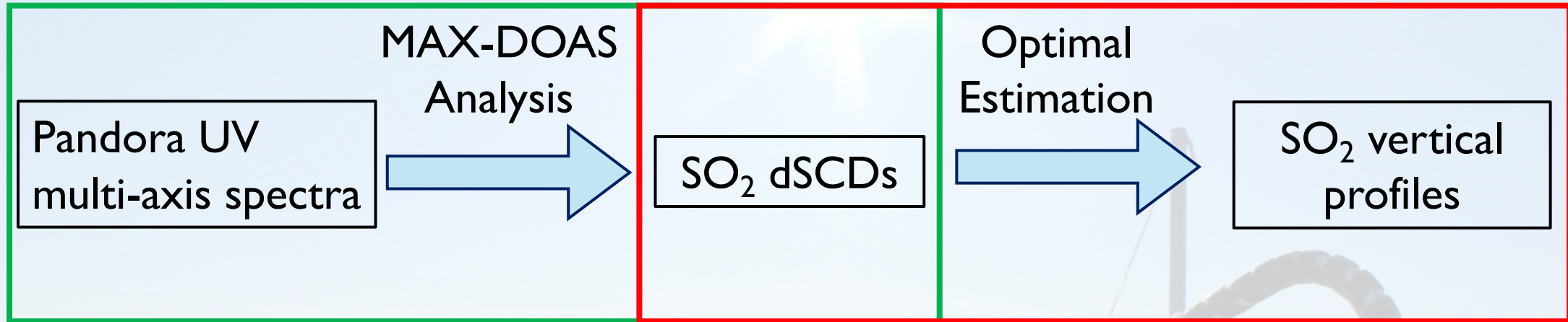
Retrieval settings  
from Wang  
et al. (2014)



# Case Study I: SO<sub>2</sub> dSCDs at Izana

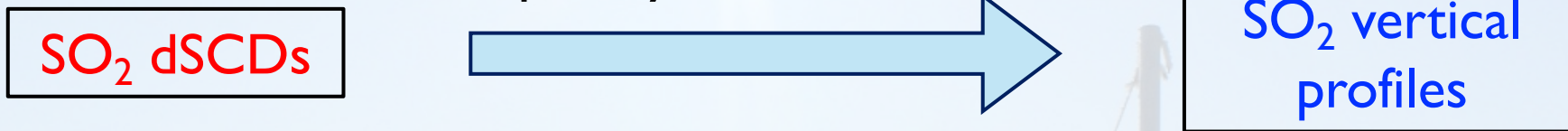


# Next: SO<sub>2</sub> dSCDs to SO<sub>2</sub> Profiles



# Next: SO<sub>2</sub> dSCDs to SO<sub>2</sub> Profiles

Optimal Estimation algorithm:  
Mexican Maxdoas Fit (MMF),  
developed by Martina M. Friedrich



Run through the radiative transfer  
model VLIDORT v2.7

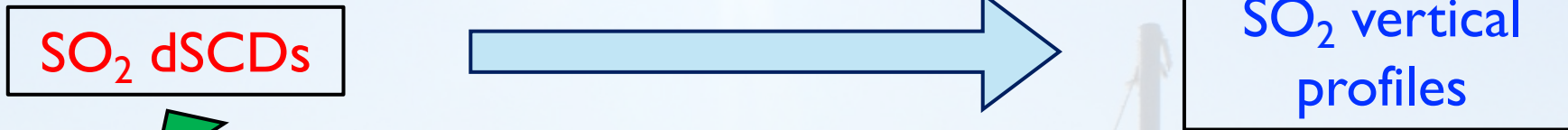
$$\mathbf{y} = F(\mathbf{x}, \mathbf{b}) + n$$

Get modelled  
dSCD output

Start with a priori SO<sub>2</sub> profile  
(exponentially decreasing profile with  
 $H=0.5$  km...this was challenging!)

# Next: SO<sub>2</sub> dSCDs to SO<sub>2</sub> Profiles

Optimal Estimation algorithm:  
Mexican Maxdoas Fit (MMF),  
developed by Martina M. Friedrich



Compare differences

Run through the radiative transfer  
model VLIDORT v2.7

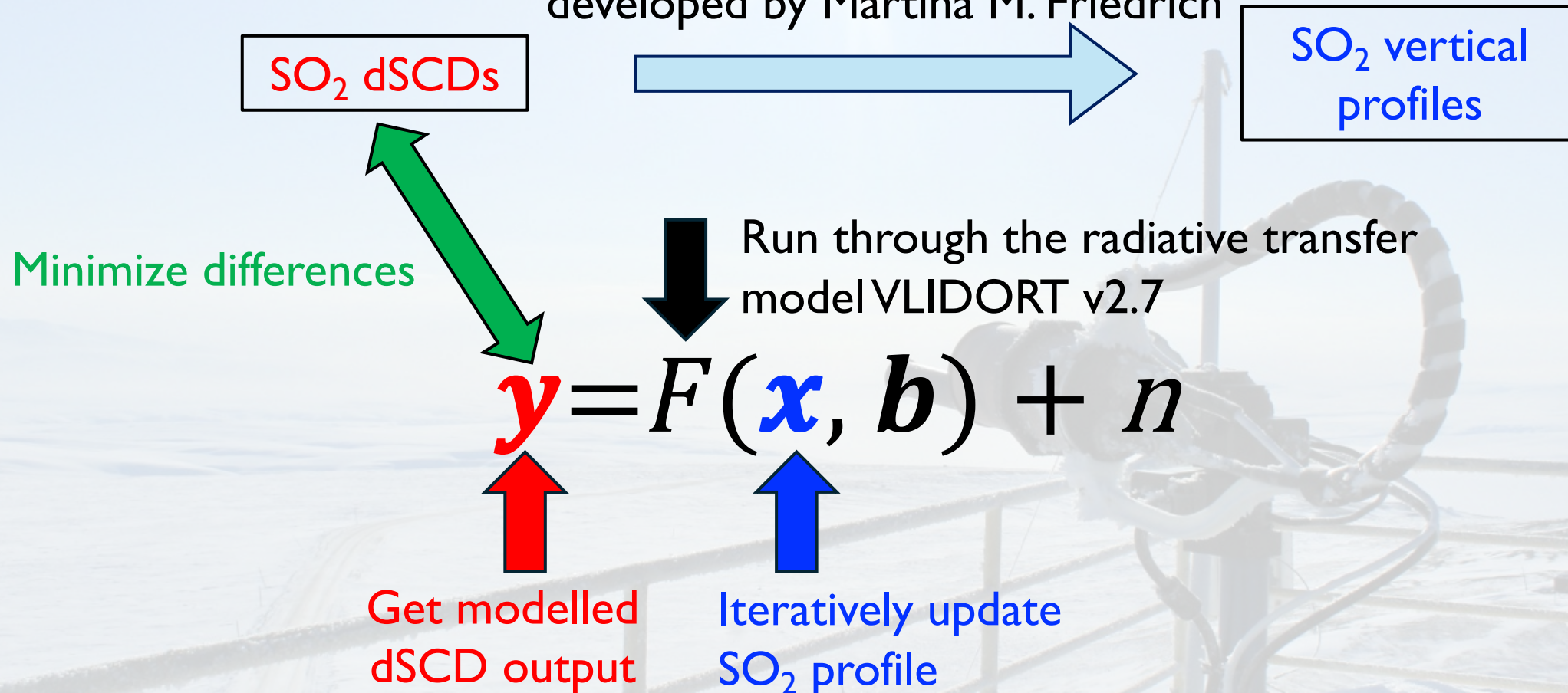
$$y = F(x, b) + n$$

Get modelled  
dSCD output

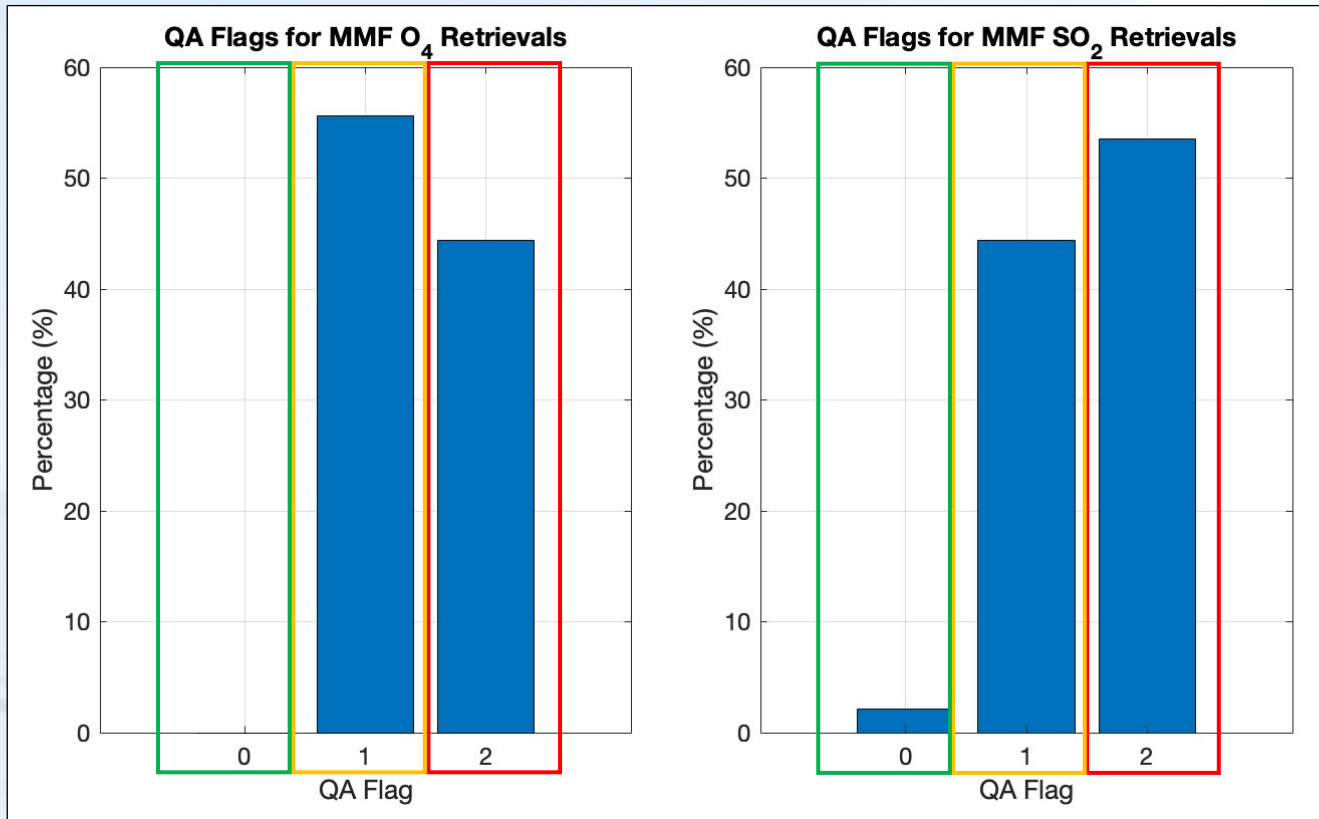
Start with a priori SO<sub>2</sub> profile  
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# Next: SO<sub>2</sub> dSCDs to SO<sub>2</sub> Profiles

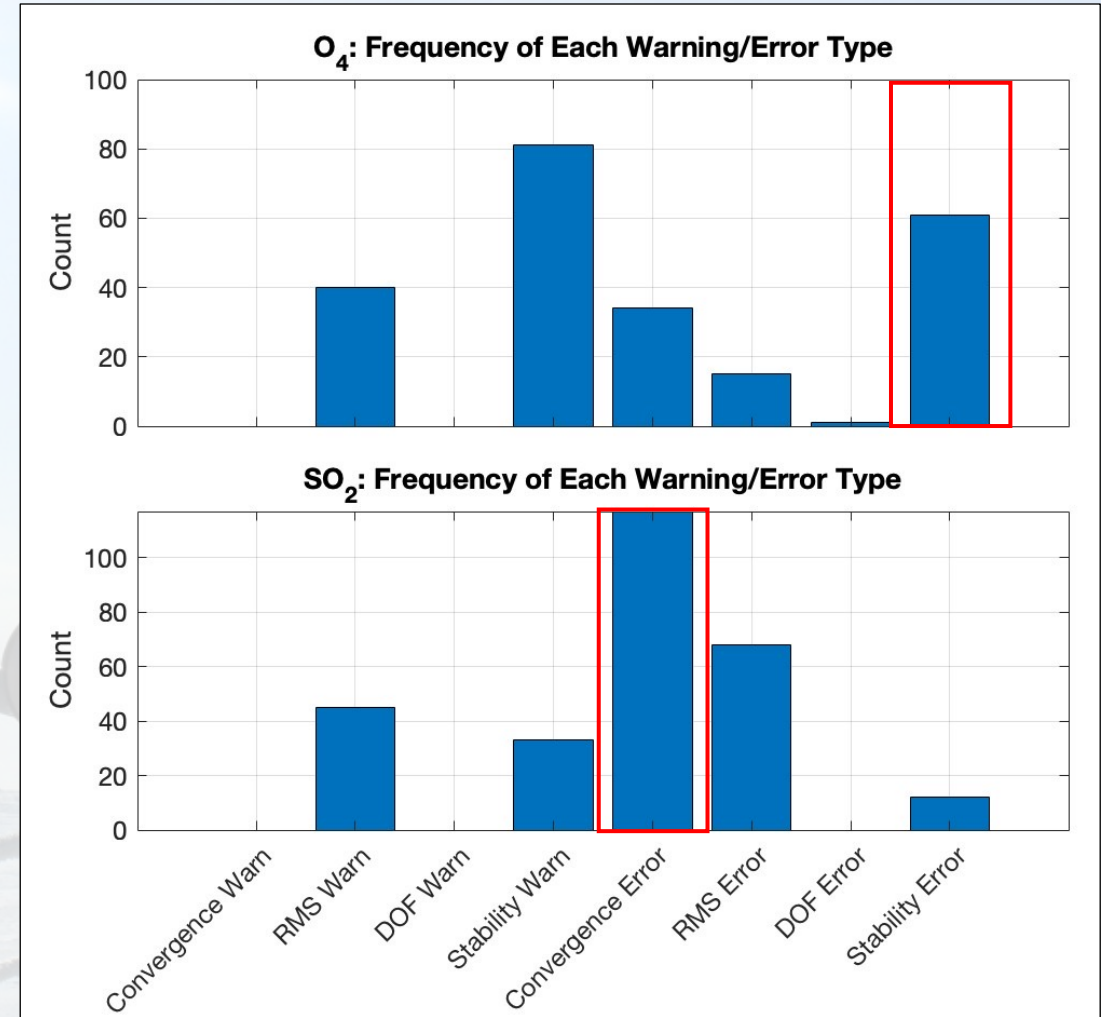
Optimal Estimation algorithm:  
Mexican Maxdoas Fit (MMF),  
developed by Martina M. Friedrich



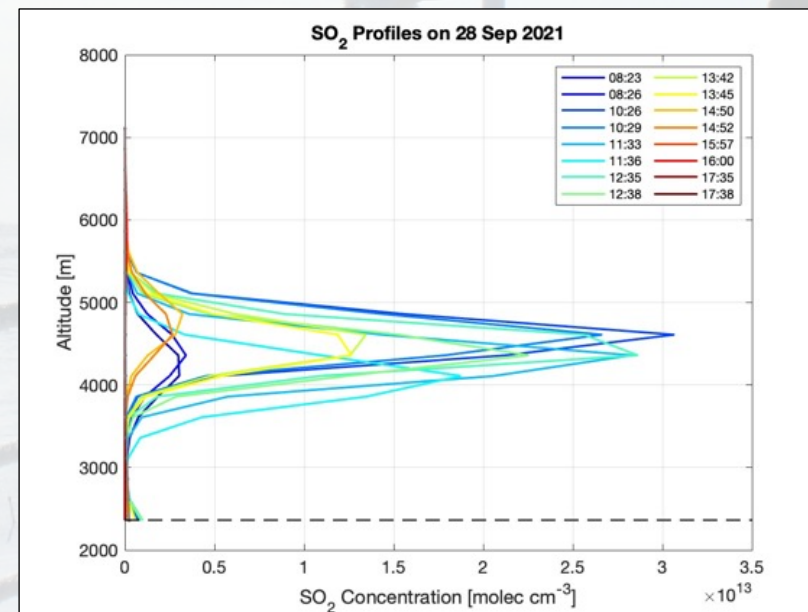
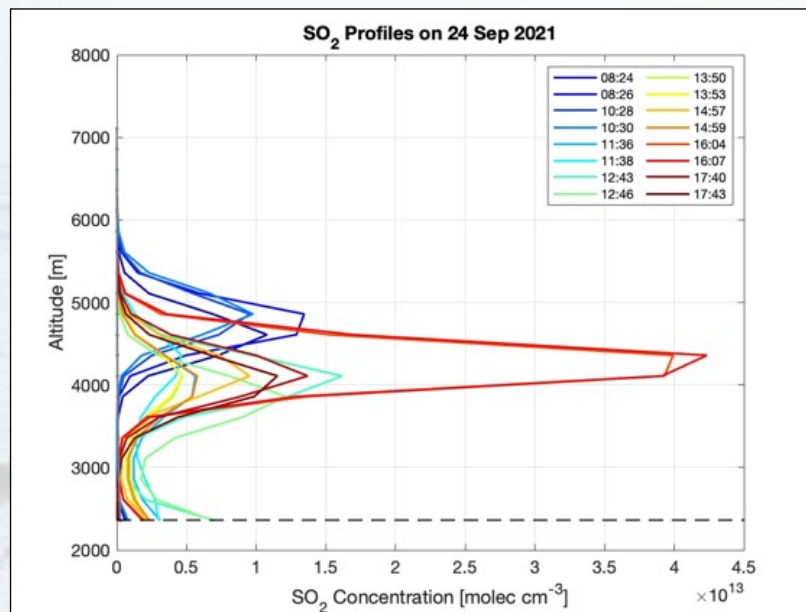
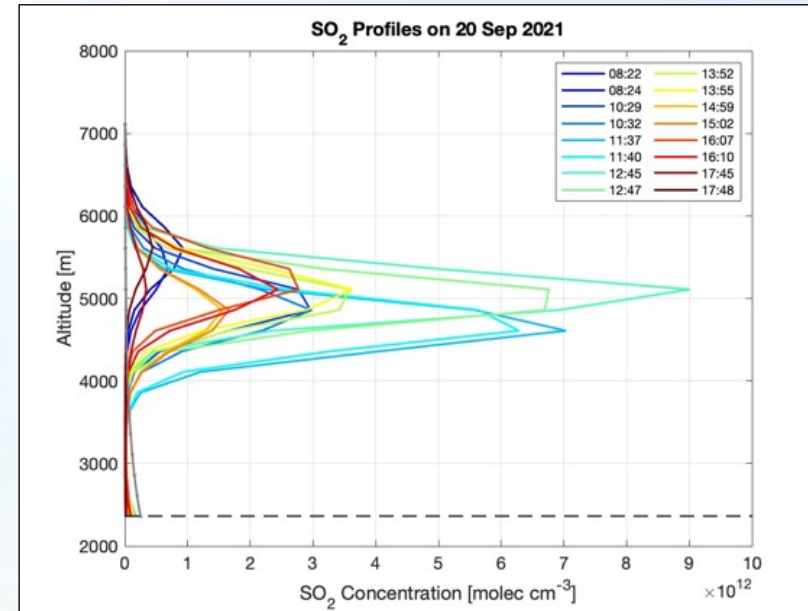
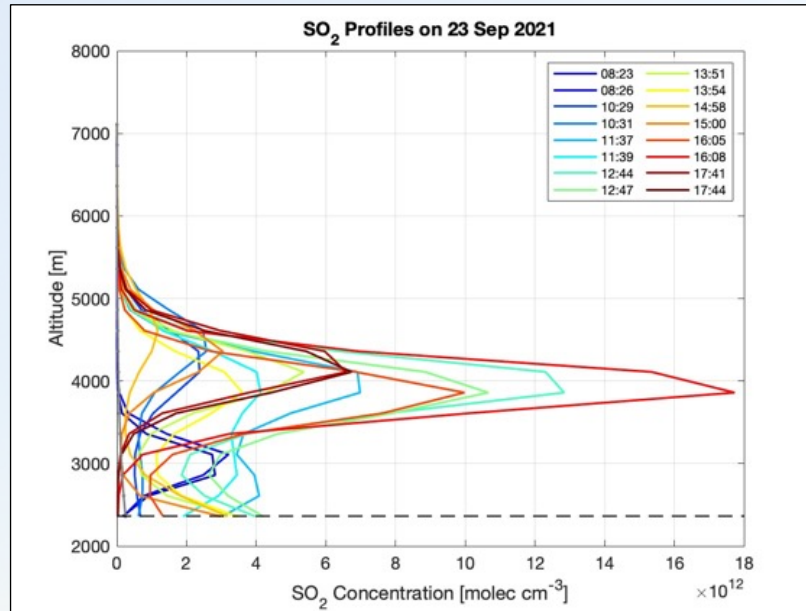
# Results: SO<sub>2</sub> Profiles at Izana



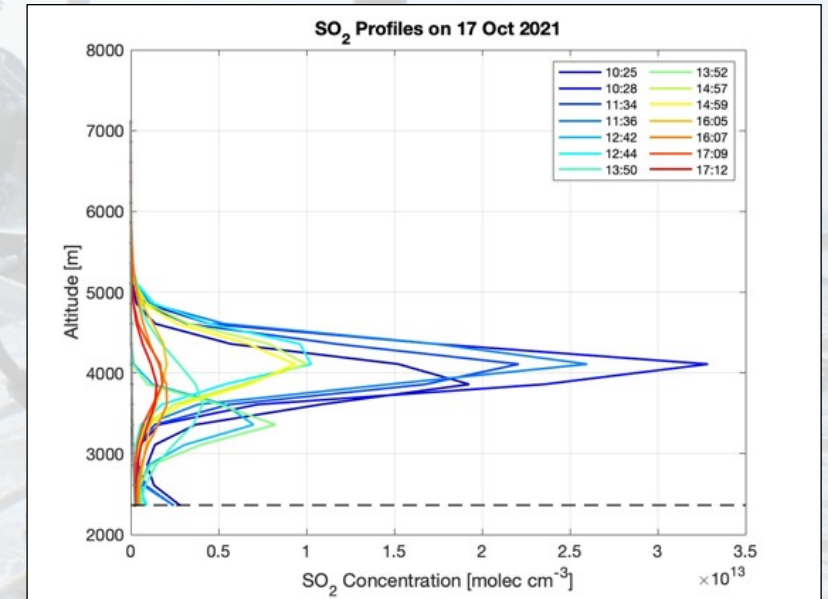
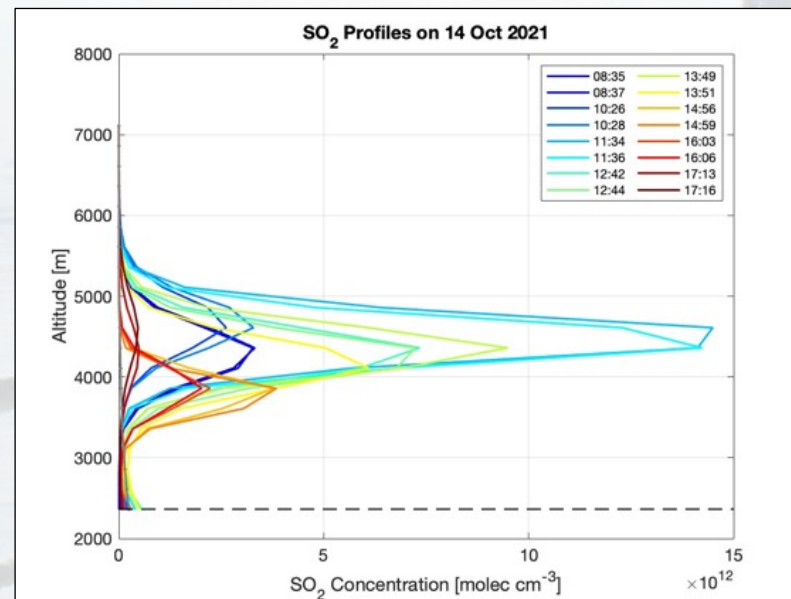
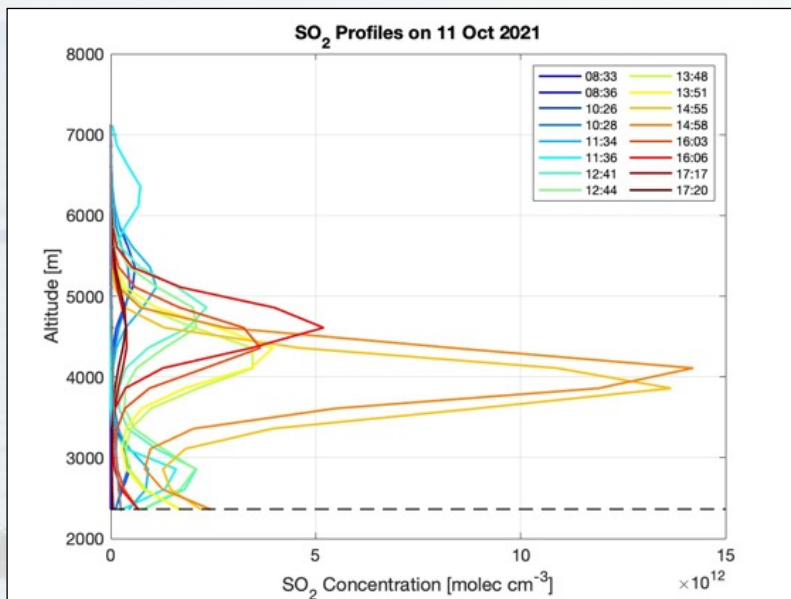
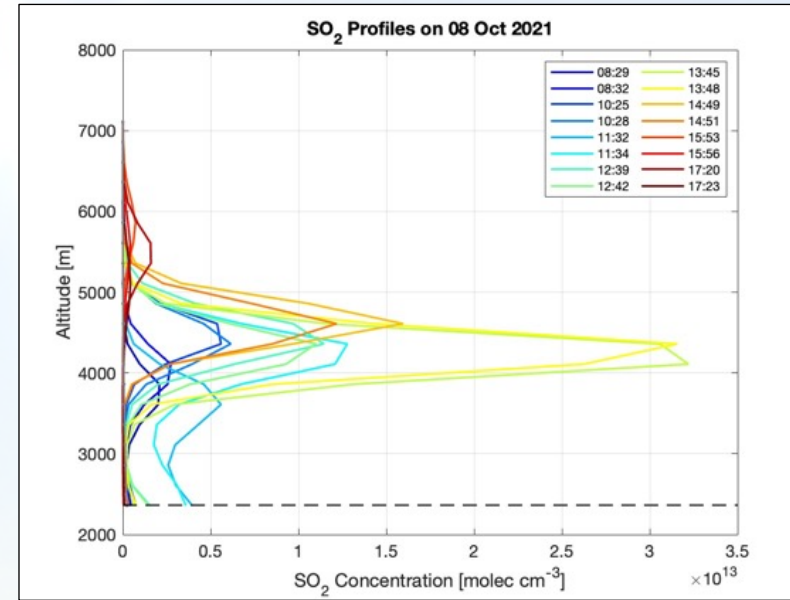
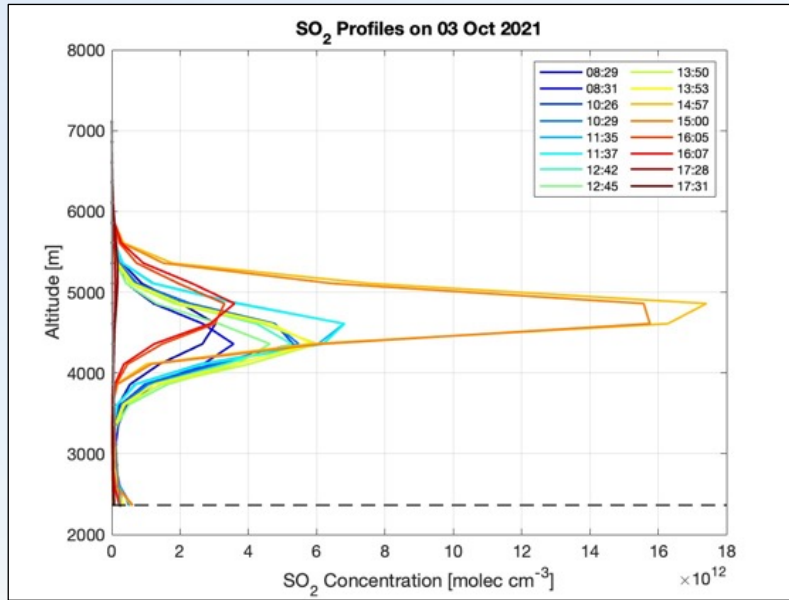
No warnings or errors   Warning   Error



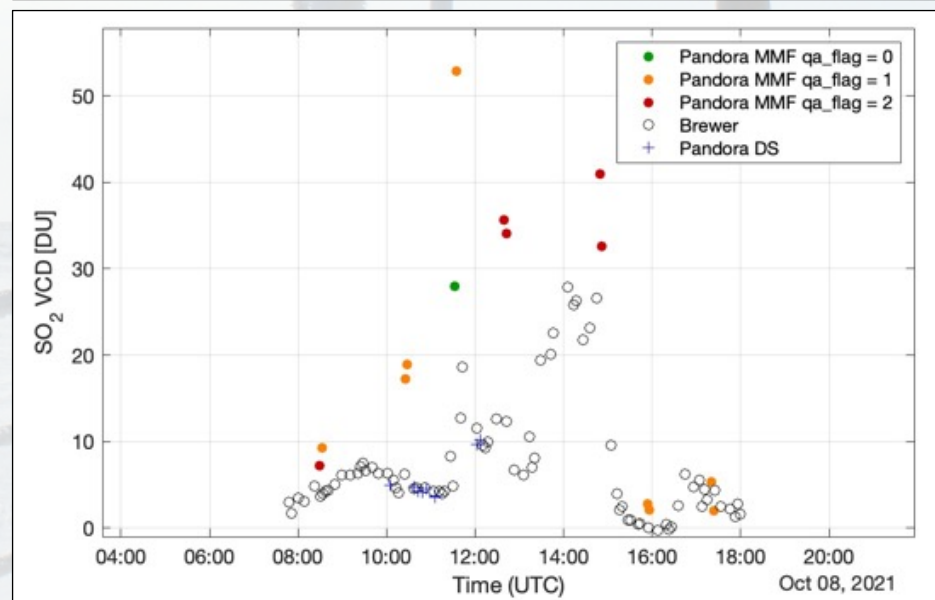
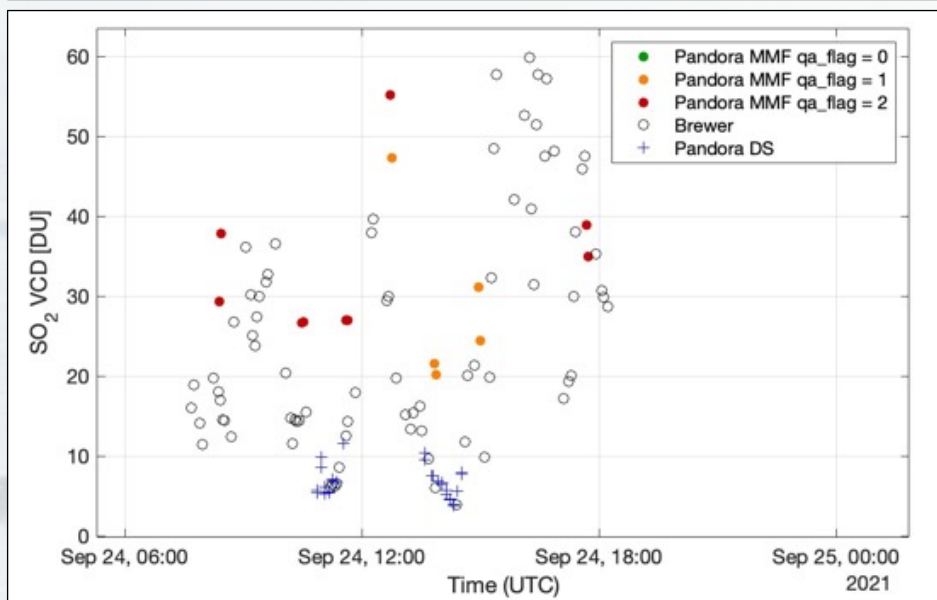
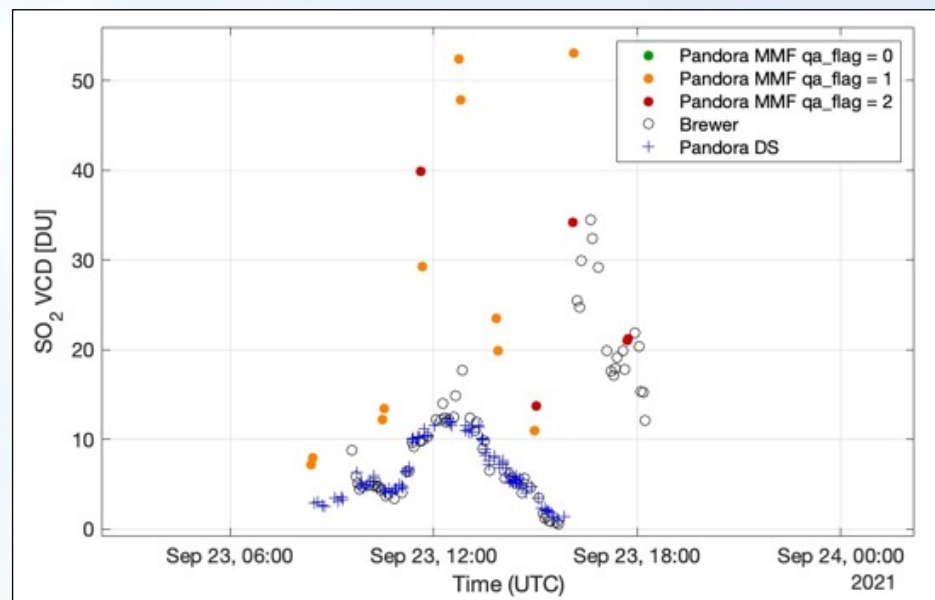
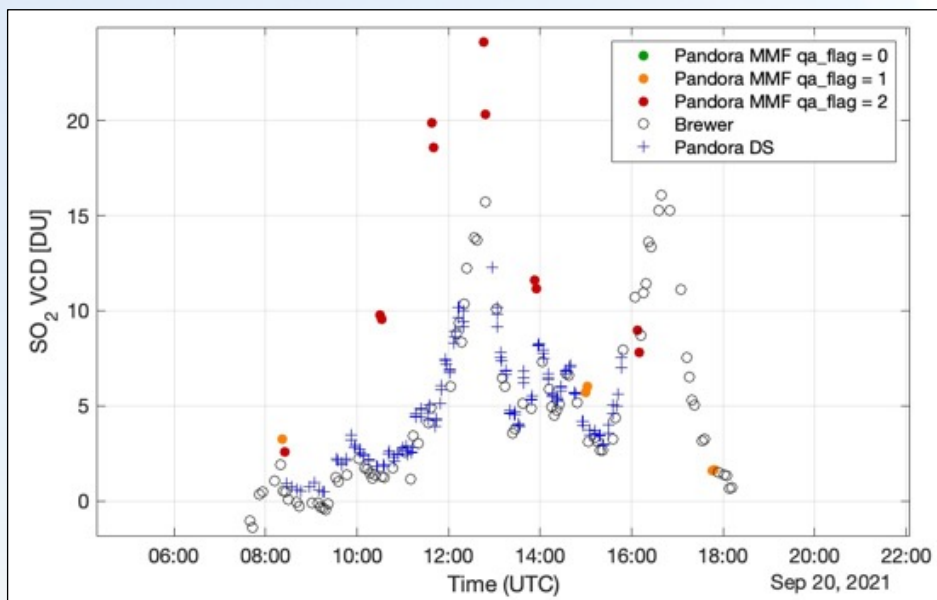
# Results: SO<sub>2</sub> Profiles at Izana (Sept 2021)



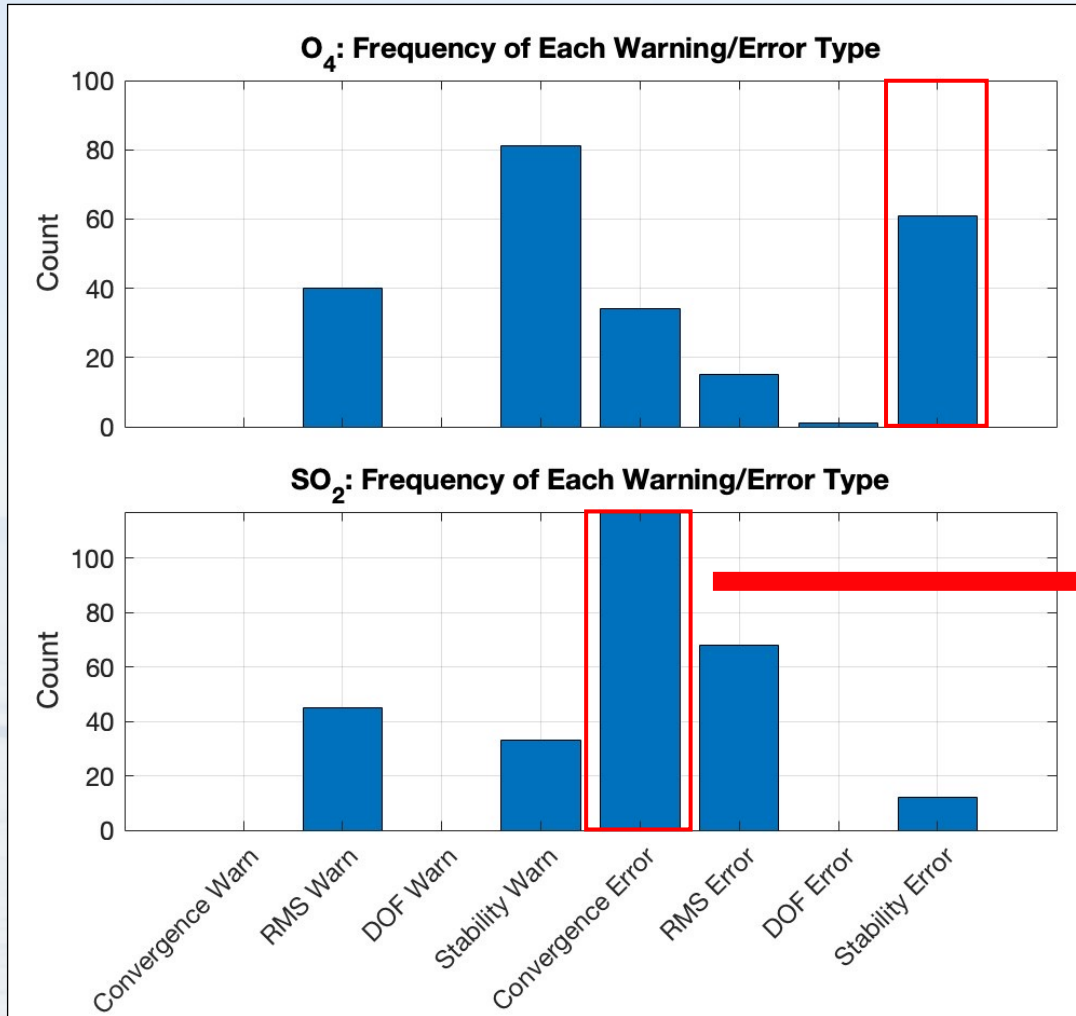
# Results: SO<sub>2</sub> Profiles at Izana (Oct 2021)



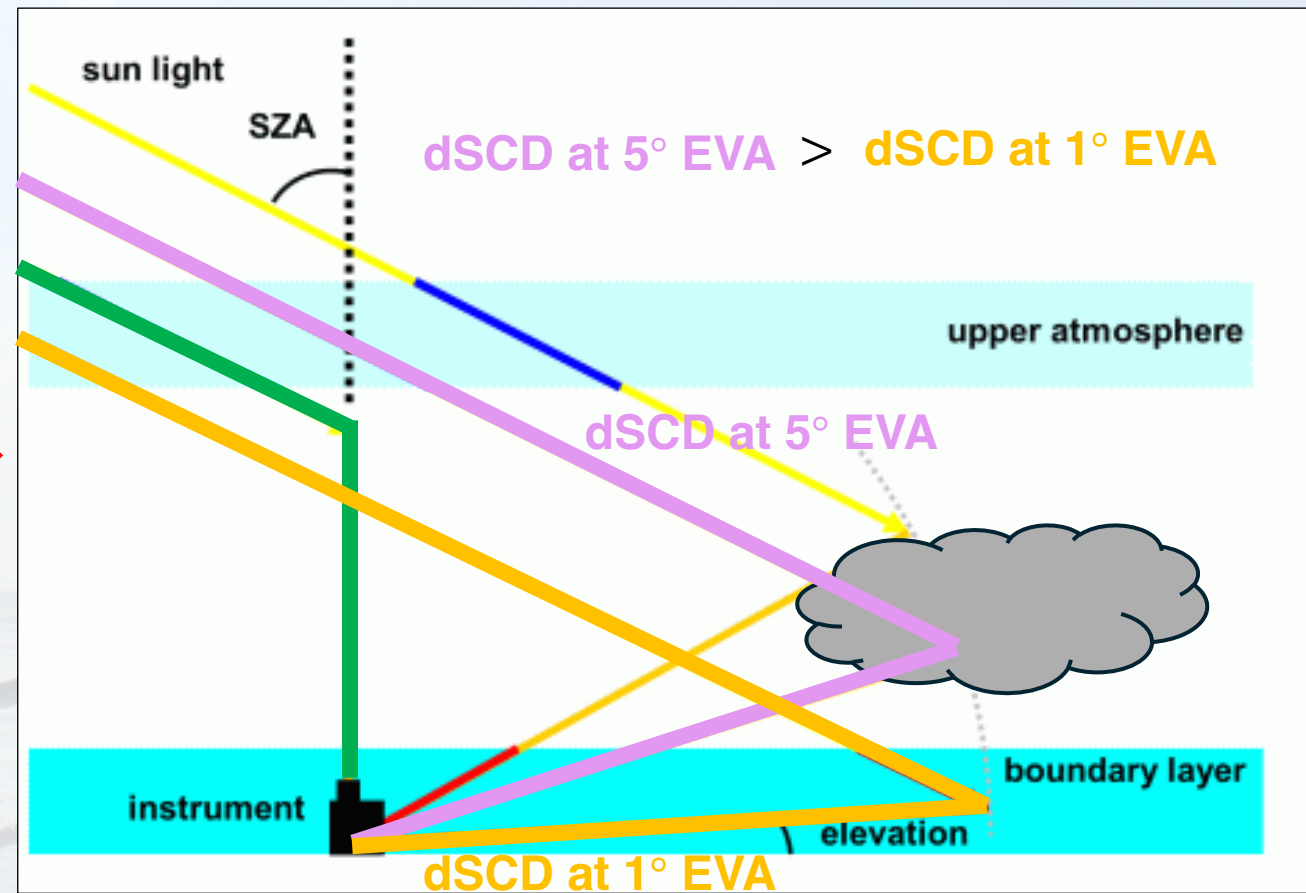
# Results: SO<sub>2</sub> VCDs at Izana (Sept to Oct 2021)



# Results: SO<sub>2</sub> Profiles at Izana

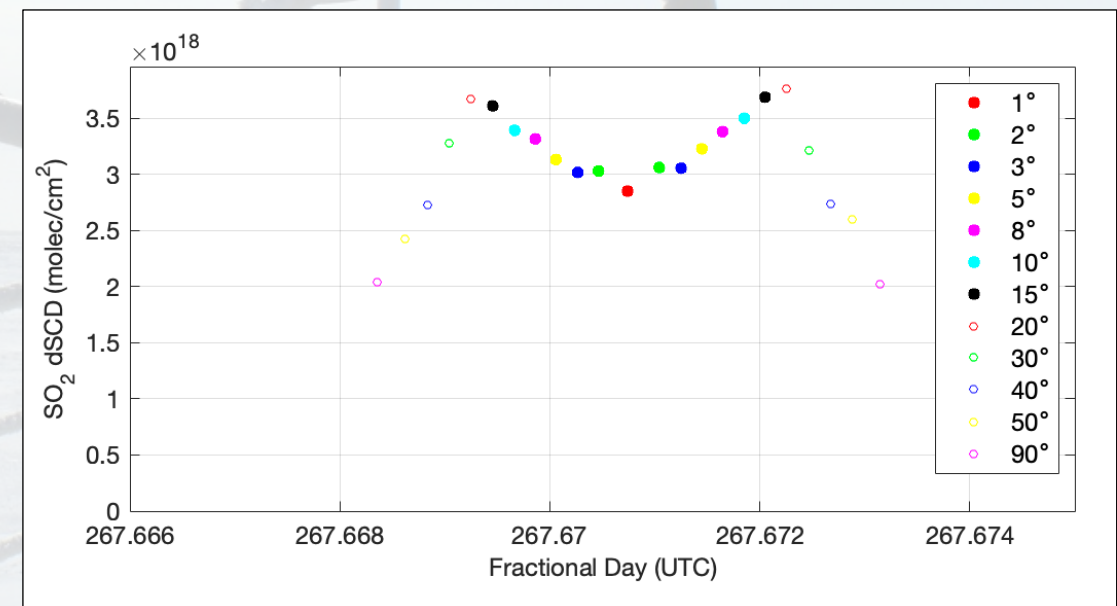
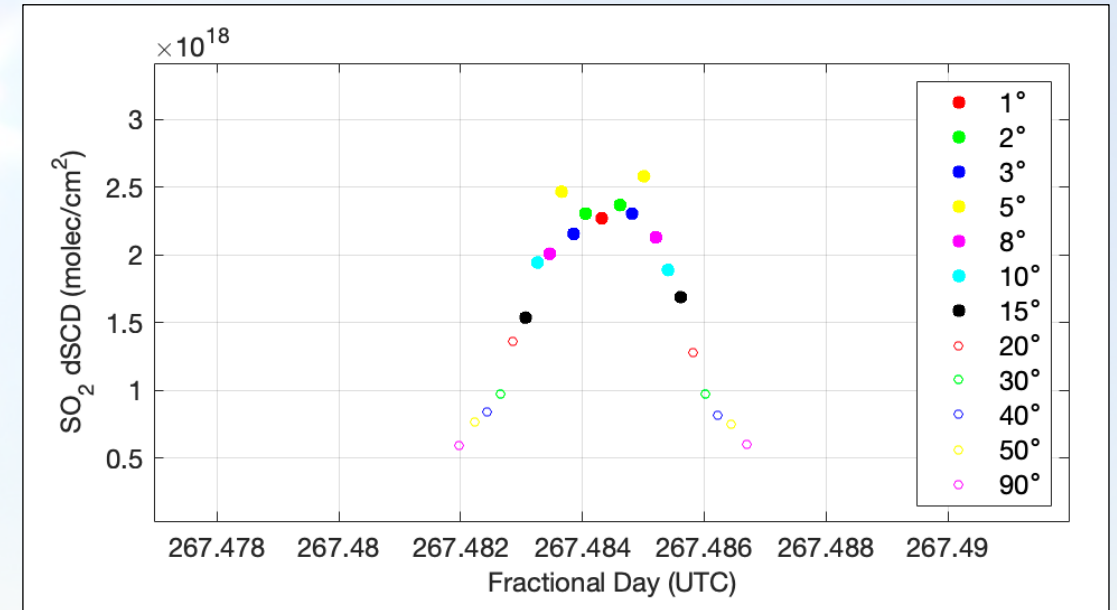
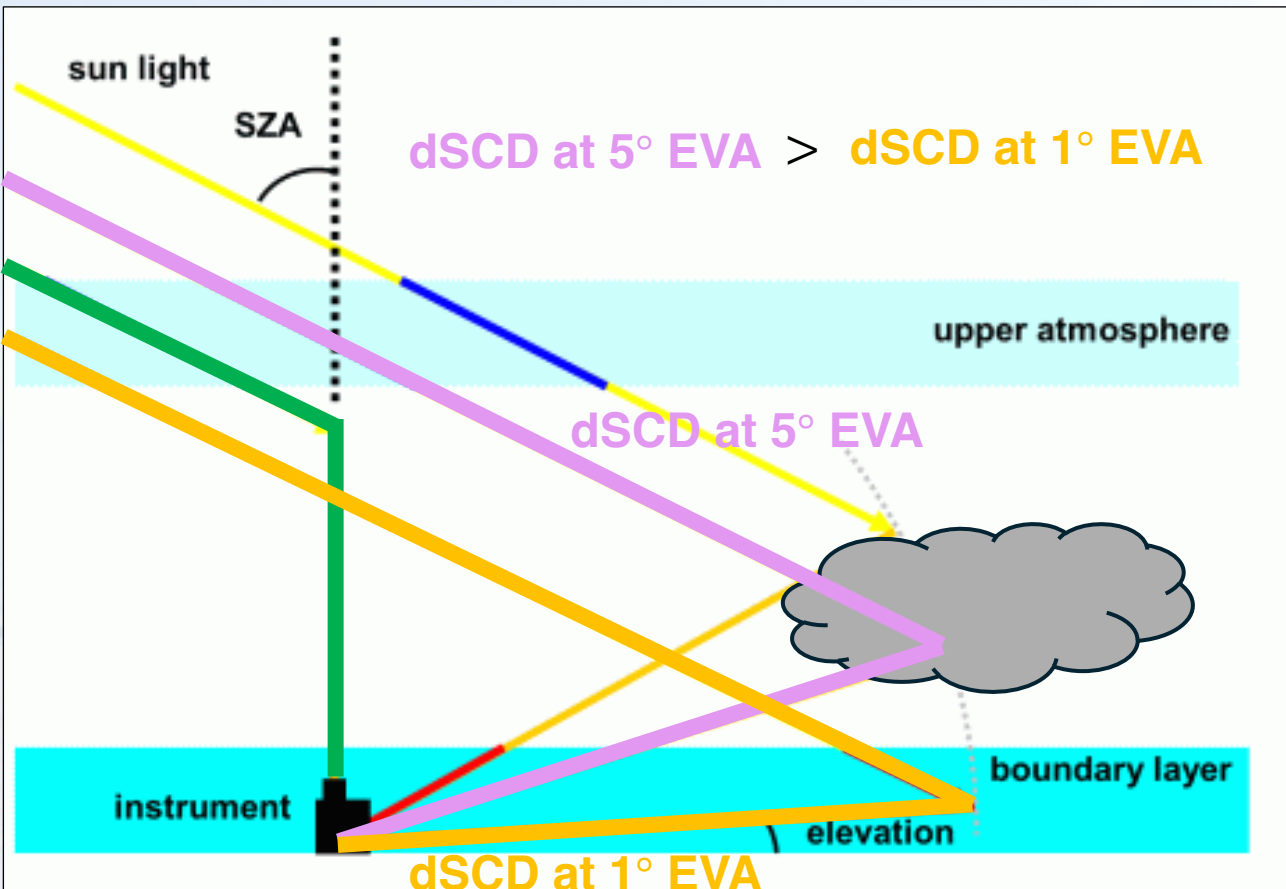


Horizontal inhomogeneity  
in SO<sub>2</sub> field along line of sight?

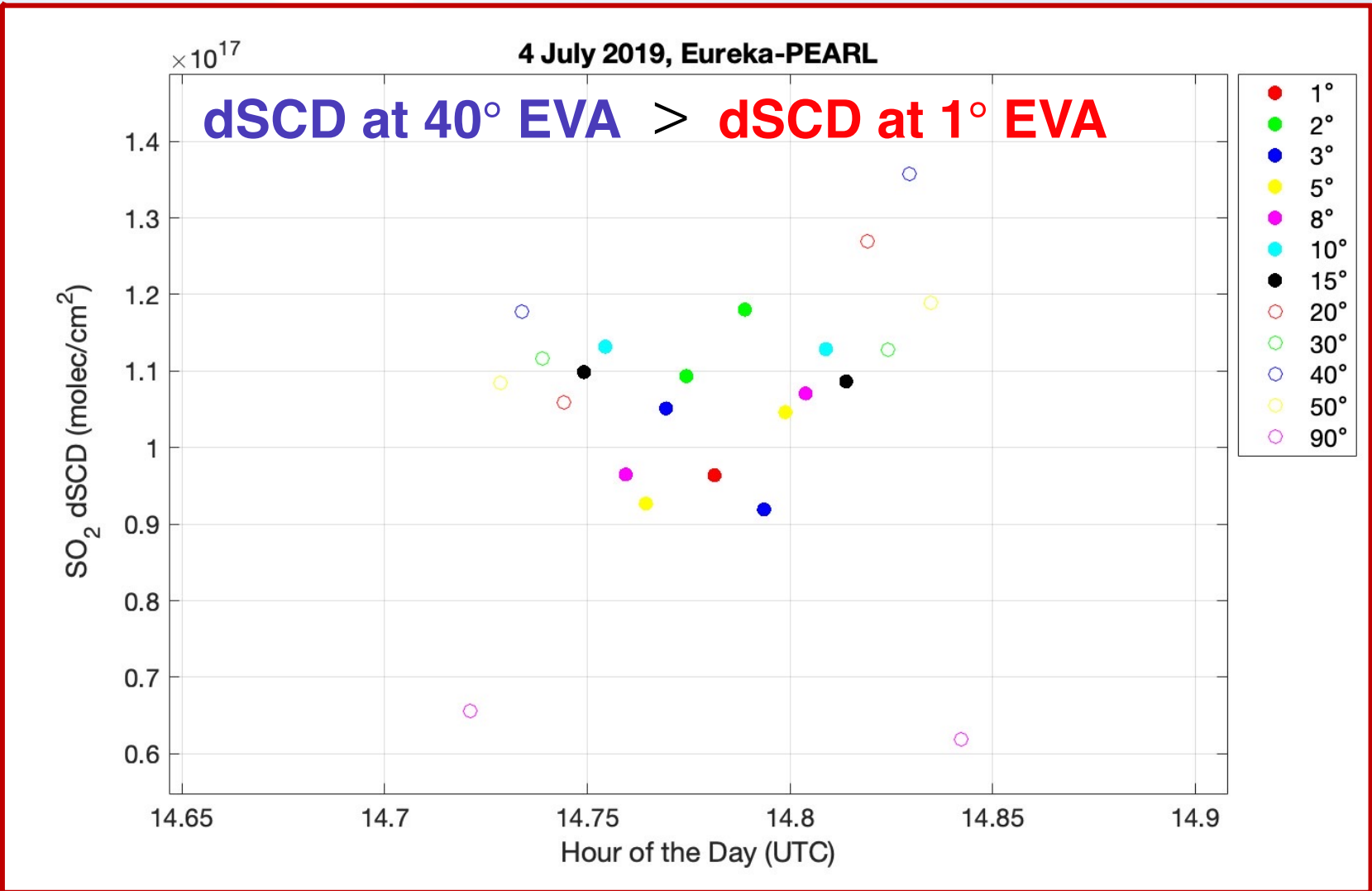
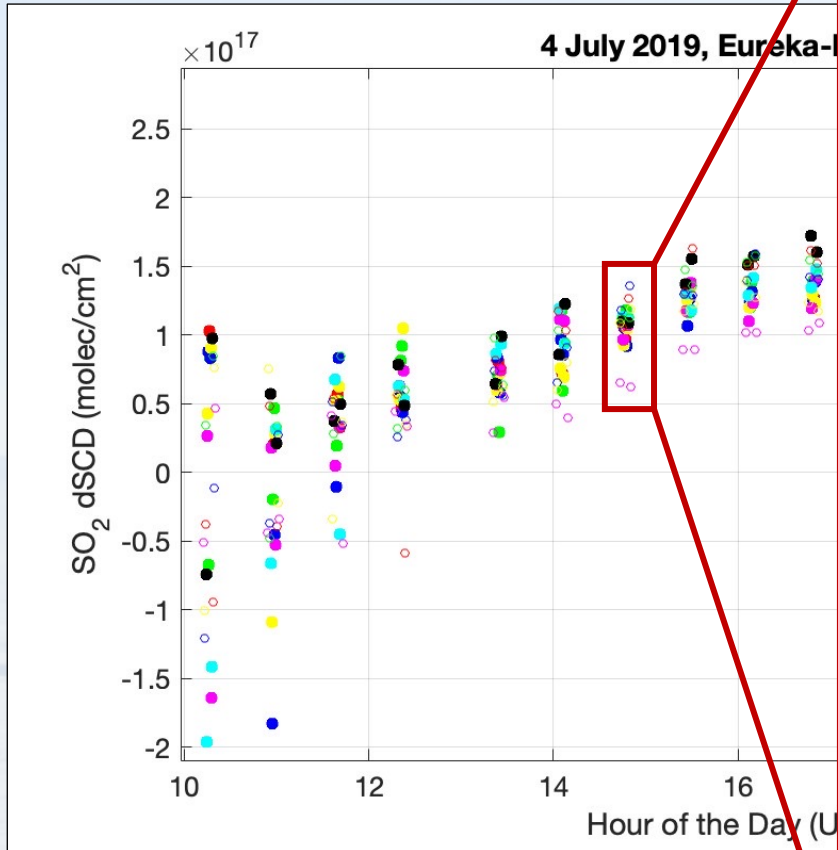


# Results: SO<sub>2</sub> Profiles at Izana

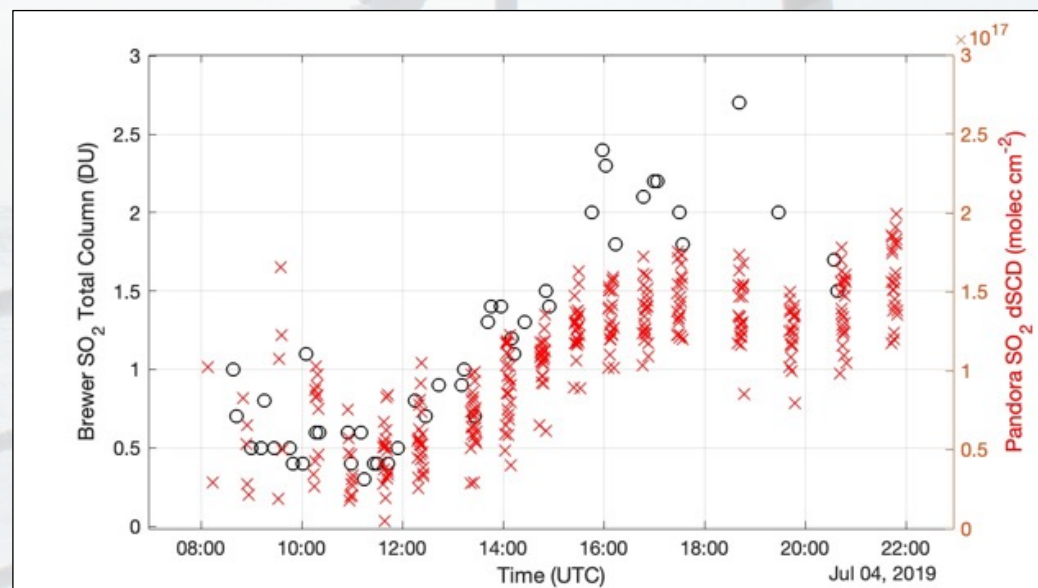
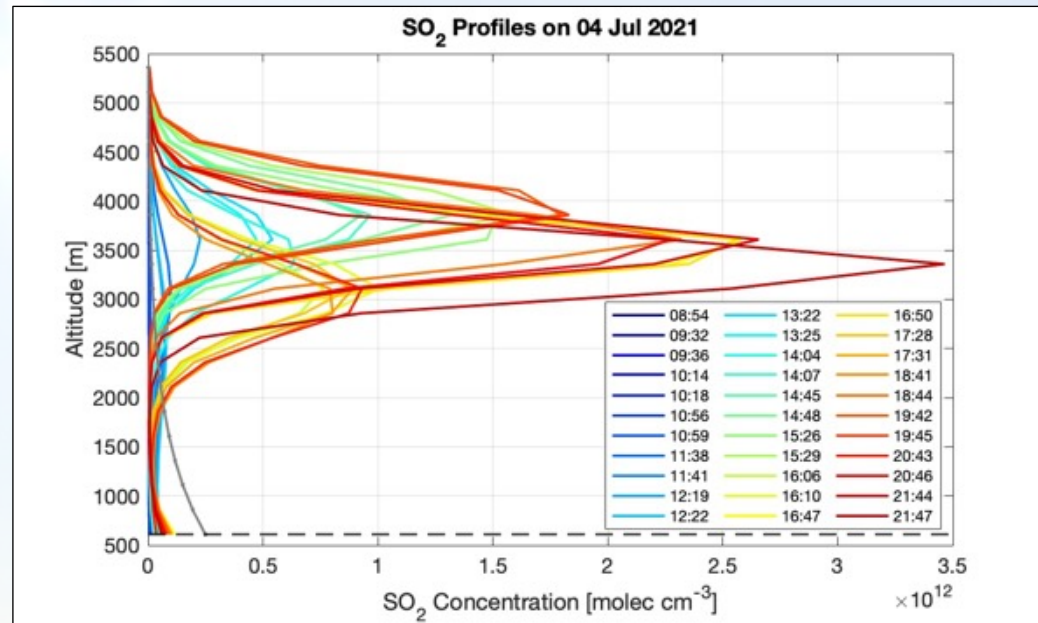
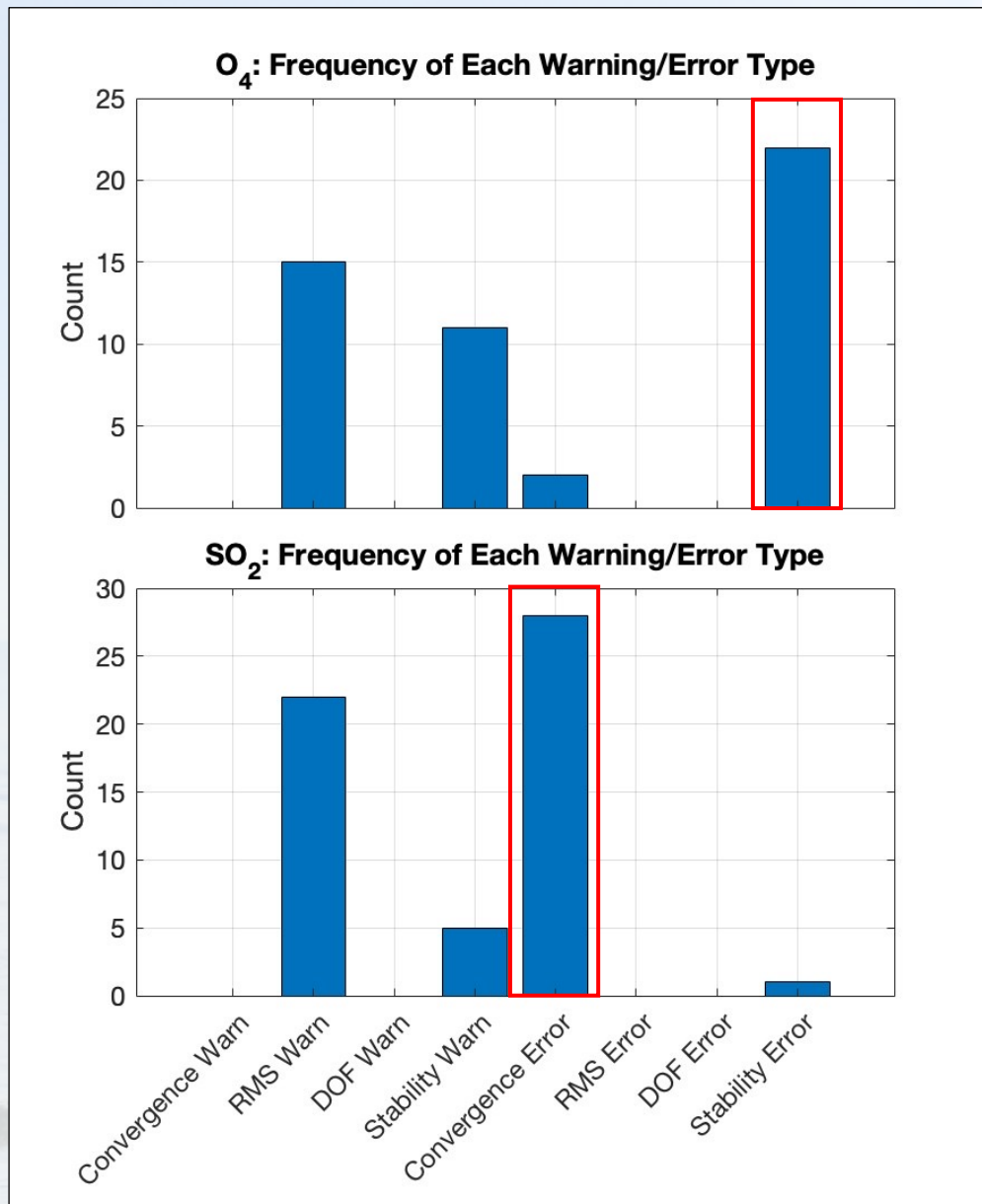
Horizontal inhomogeneity  
in SO<sub>2</sub> field along line of sight?



# Case Study 2: SO<sub>2</sub> dSCDs at Eureka-PEARL



# Results: SO<sub>2</sub> Profiles at Eureka-PEARL (4 July 2019)



# Pandora SO<sub>2</sub> Profiling: Future Work

- **SO<sub>2</sub> dSCDs**
  - Can QDOAS settings be further optimized?
- **SO<sub>2</sub> Profiles**
  - Can profile results be obtained with predominantly no errors?
  - How do the profiles compare to satellite measurements of SO<sub>2</sub> layer heights, in situ surface SO<sub>2</sub>, and ground-based SO<sub>2</sub> columns?
- Can this work be expanded to more PGN sites, such as sites with anthropogenic SO<sub>2</sub>?

# PGN Sites with Elevated SO<sub>2</sub>

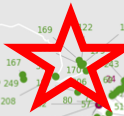
PI44 at Eureka-PEARL



PI47 at SWDetroit

P39 at DearbornMI

P208 at WindsorWest



P101 at Izana



P216 at Ulaanbaatar



PI42 at MexicoCity-UNAM

PI57 at MexicoCity-Vallejo

P65 at Alzomoni



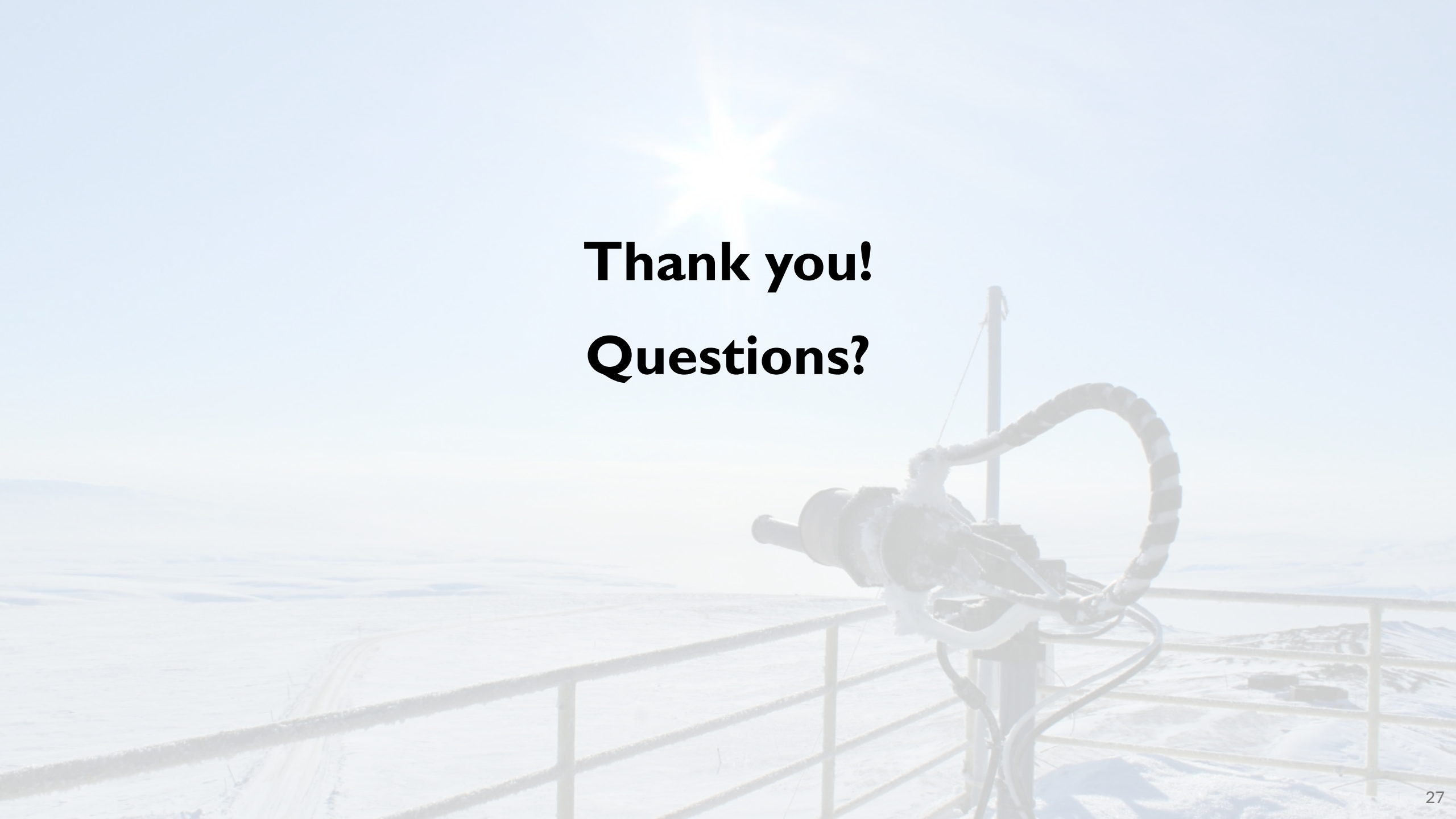
PI59 at Wakkerstroom



P211 at Agam



- PGN status
- |           | official | non official |
|-----------|----------|--------------|
| real time |          |              |
| delayed   |          |              |

A bright sun in a clear blue sky over a snowy landscape with a metal railing and a camera-like device in the foreground.

**Thank you!**  
**Questions?**