CTAO

UNIVERSITÉ
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FACULTÉ DES SCIENCES

Molecular atmospheric uncertainties and characterisation at CTAO

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Introduction

Atmosphere is the medium with which γ-rays interact and Cherenkov light is produced and propagates

- **Atmospheric molecular density**
  - Longitudinal shower development, height of first interaction, intensity of Cherenkov light
- **Refractive index profile**
  - Cherenkov light production threshold, emission angle
- **Light transmission**
  - Extinction = absorption + scattering
  - <u>Molecular extinction</u>
    - Rayleigh scattering + absorption (mainly O_3)
  - <u>Aerosol extinction</u>
    - Clouds, aerosols

Objective

Ongoing effort to estimate CTAO systematic uncertainties budget

- Atmosphere affects energy estimation, flux estimation, and source localization
- CTAO has set stringent requirements for systematic uncertainties, e.g. for energy estimation:

$$\left(\frac{\delta E_{scale}(E)}{E}=10\,\%\right)\sim\left(\frac{\delta E_{atmosphere}(E)}{E}=8\,\%\right)\oplus\left(\frac{\delta E_{telescopic\ part}(E)}{E}=5\,\%\right)\oplus\left(\frac{\delta E_{analysis}(E)}{E}=4\,\%\right)$$

- Significant improvement wrt current IACTs (~15% under optimal conditions)

Objective: understand and reduce systematic uncertainties related to the molecular atmosphere

- Atmospheric monitoring & characterisation
  - Molecular atmosphere calibration suite

Shower development & Cherenkov light creation

Observations from past studies* have shown

- Cherenkov light density on the ground can vary up to 60% for atmospheric models of different geographical latitudes.
- Seasonal variations of mid-latitude models show differences in the range of 5-15%.

These variations highlight the need for detailed molecular atmosphere characterization

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K. Bernlöhr Astroparticle Physics 12 (2000) 255–268
P. Munar-Adrover and M. Gaug, European Physical Journal Web of Conferences. Vol. 197. European Physical Journal Web of Conferences. Sept. 2019, p. 01002
M. K. Daniel. “Application of radiosonde data to VERITAS simulations”

Molecular atmosphere characterisation pipeline

First implementation of the molecular atmosphere characterisation suite

- It calculates the astronomical dusk and dawn → timeseries to be requested
- It requests & retrieves the timeseries of meteorological data from Data assimilation Systems (DAS)
- Analyses the meteorological data & produces a profile describing the atmosphere state for the given night

2 modes of operation

The Calibration Pipeline can produce a contemporary model describing the atmosphere over the observatory for any given night that contains all the required information in order to launch Corsika simulation

    - Production of tailored IRFs for a given observation

The Calibration Pipeline can select a seasonal model best matching the conditions over the observatory for a given night

- The selection is based on the molecular number density at an altitude of 15km a.s.l.
  - Selection of the best matching set of pre-calculated IRFs

Molecular atmosphere calibration input data

DAS reanalysis / analysis datasets

- DAS provide datasets over a grid covering Earth, at various pressure levels for each grid point. Datasets are updated every (few) hours
- Dataset become publicly available with some latency

GDAS ds083.2, available from Research Data Archive

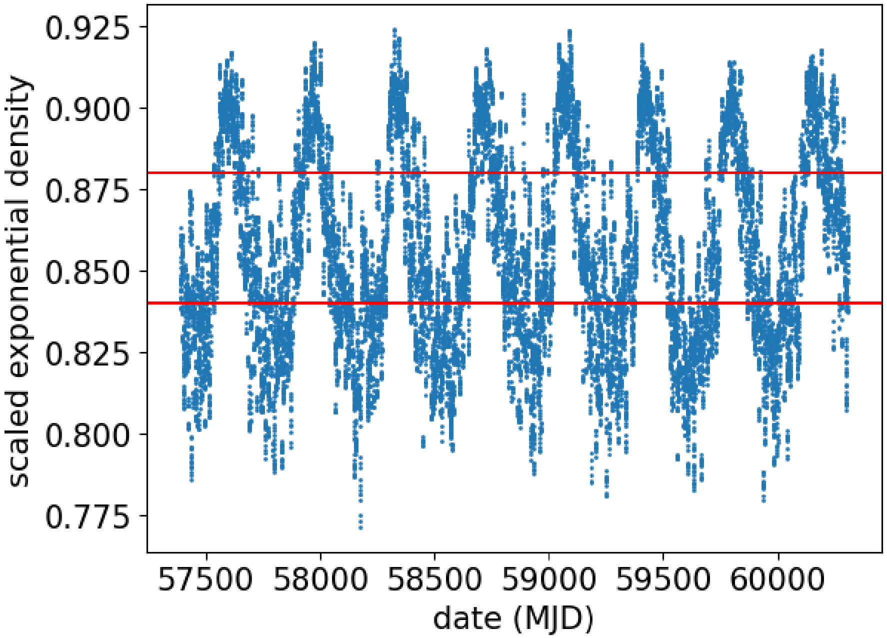
- Few hours latency, 120km x 120km grid, update every 6 hours, ceiling ~ 26 km a.s.l. rather unstable interface

ECMWF ERA-5, available from Copernicus (EU program)

- 5 days latency, 31km x 31km grid, update every hour, ceiling ~45km a.s.l., stable interface

Available grid from Copernicus

Seasonal profiles uncertainties



Variations of molecular density at 15km a.s.l. during 8 years in La Palma. The data comes from the analysis of ERA5 dataset of ECMWF, available through Copernicus. We can see 3 seasons.

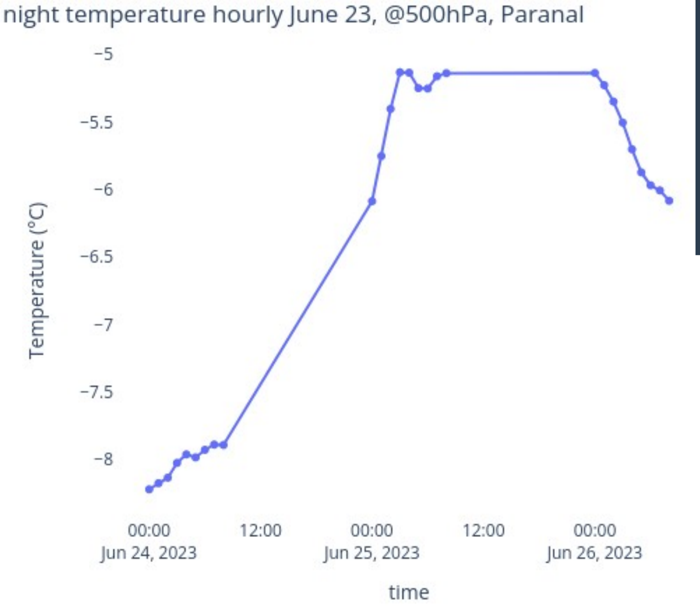
An uncertainty of ~5% has been estimated for the North in previous studies if no molecular atmosphere calibration is applied.

- It can be reduced to ~3% with the use of seasonal models.

Ongoing studies

- Season definition & uncertainty budget estimation for the South site
- Refinement of the uncertainty budget for the North site using latest years data retrieved from the more precise ERA-5 dataset

Tailored profiles uncertainties

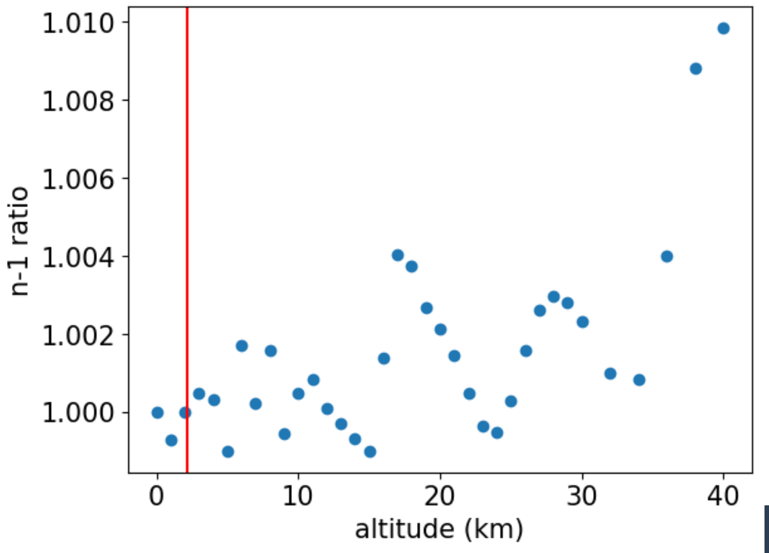


Tailored profiles should provide smaller uncertainties than seasonal ones, but:

- How can we estimate the uncertainties of the data assimilation systems?
  - According to their documentation, uncertainties either are not publicly available (GDAS-RDA) or shouldn’t be taken at face value (ECMWF)

An estimation of the systematics introduced by nightly profiles can be made by looking at the hourly variation

- It includes both DAS uncertainty + diurnal variations
  - Both constitute systematic error for nightly profiles



Data assimilation systems validation

Data assimilation systems provide the atmospheric parameters on grid points over the globe

- Can we be sure that propagating the atmospheric state to the observatory site does not introduce biases?
    - Will be translated into IRF biases
- Especially when the measurement sites are far from the observatory sites
    - South site: the closest radiosonde station is at the sea coast

Ground validation with the weather station

Even better, validation with a radiosonde campaign performed on site

Cherenkov light transmission: extinction mechanisms

Light extinction in atmosphere

Slow component:
Molecular extinction

Rayleigh scattering

- Produced by Calibration pipeline via the analysis of DAS data

Molecular absorption

- Mainly ozone
- If calibration needed
  - DAS data
- If not
  - Average profiles created with some radiative transfer code

Fast component:
aerosols/clouds

Rapidly varying (timescale of minutes)

Will be tackled using input of LIDAR & FRAM and historical climatological data

Cherenkov light transmission calibration

The Calibration pipeline will continuously monitoring the extinction processes

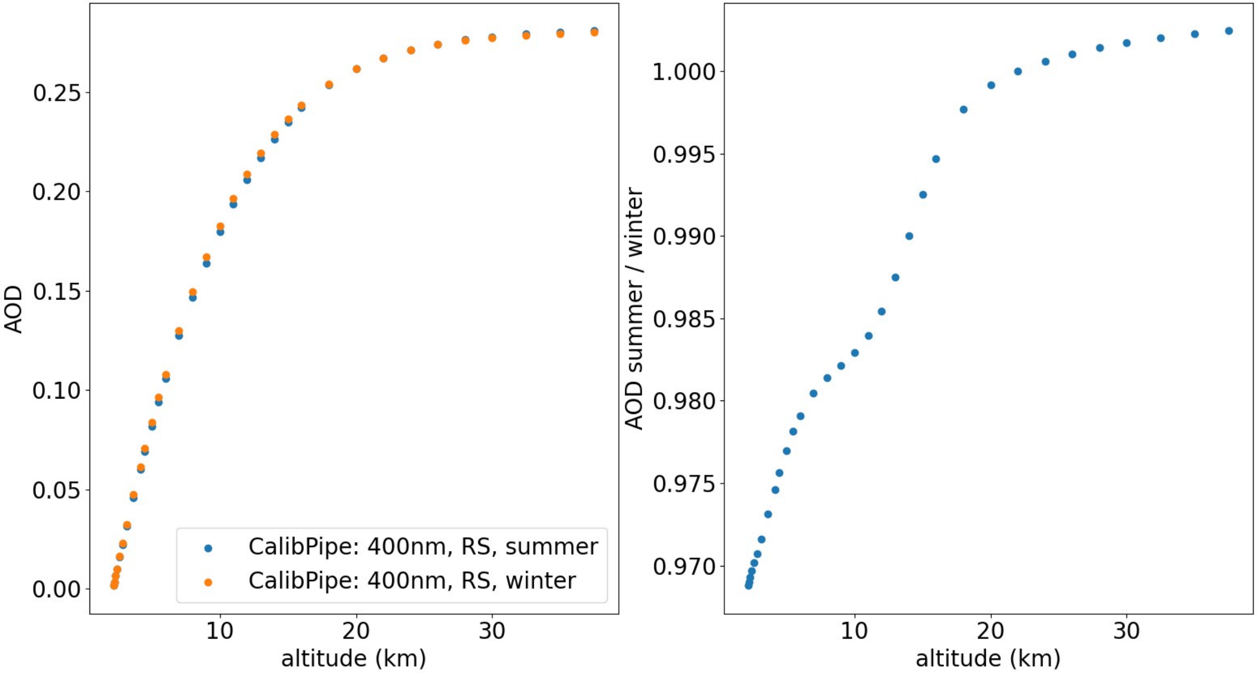
- Aerosols and clouds will be monitored via observatory elements (LIDARs & FRAMs)
- Molecular extinction via DAS (ECMWF & GDAS)?

The final calibration product will be an extinction hypercube

- Represents optical depth evolution as a function of time, wavelength, altitude, and pointing
- The fast component of the extinction hypercube will be updated during an observation block

Here we focus on the molecular extinction

Rayleigh scattering



The dominant light extinction process in a clear night

- Preliminary studies of a first version of seasonal profiles for La Palma
- The difference in the Cherenkov light density reaching the ground is within 1 %
- Simulation studies using more elaborate seasonal profiles have been planned

Ozone study: motivations

Will the use of an average ozone profile, produced with a radiative transfer code, satisfy CTAO requirements?

- There are several processes (seasonal variation, stratosphere to troposphere transport, horizontal transport of anthropogenic ozone)

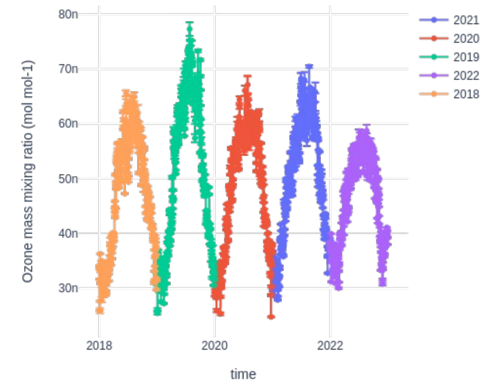
Scope of the study

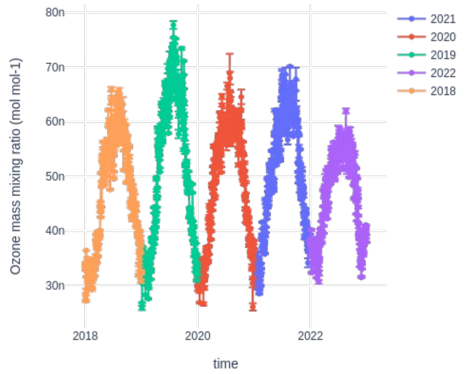
1) See if we indeed need ozone monitoring & calibration
2) If yes, with what frequency (daily, seasonal)
3) Produce software tools & workflows towards that end

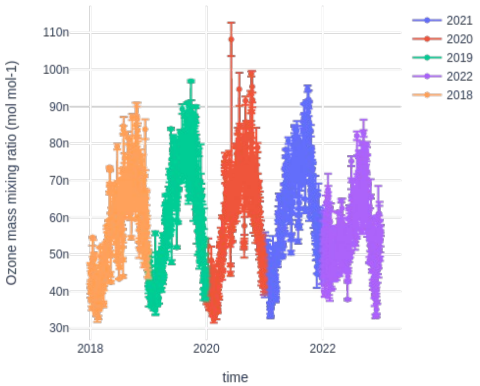
But first let’s see the variations of ozone mixing ratio at various pressure levels

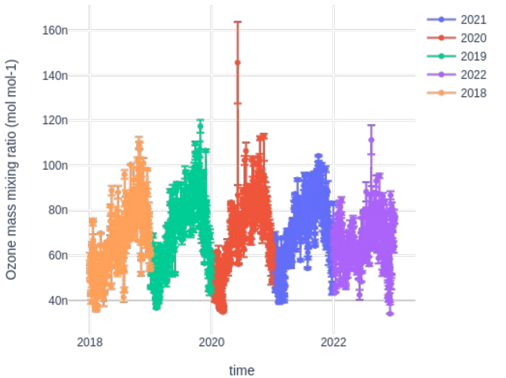
- ECMWF ERA-5 dataset, available through Copernicus, 5 years (2018-2022), over the South site
- First analysis performed at the Climate Data Store (CDS) servers, using Toolbox

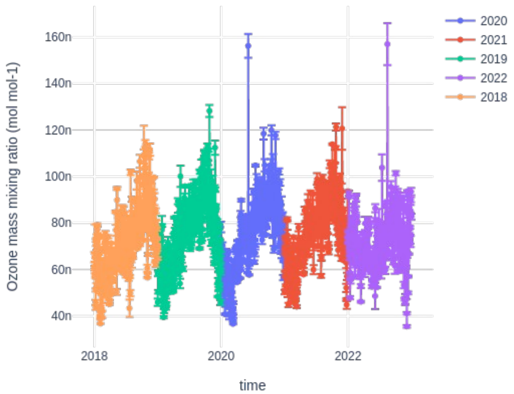
Ozone mixing ratios per pressure level (South)

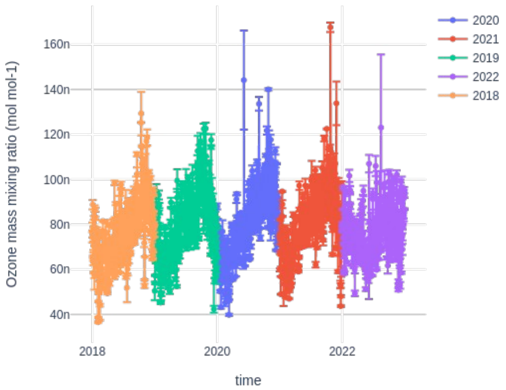

Nightly mean & std of ozone MR in Atacama @ 1000hPa

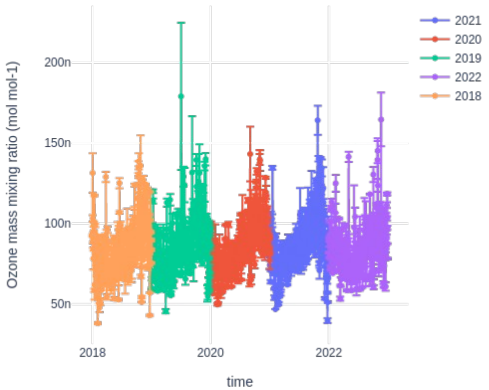

Nightly mean & std of ozone MR in Atacama @ 900hPa

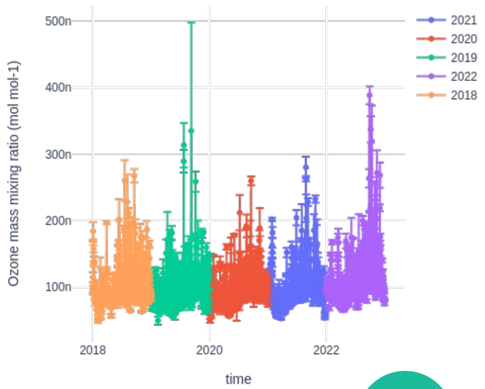

Nightly mean & std of ozone MR in Atacama @ 800hPa


Nightly mean & std of ozone MR in Atacama @ 700hPa

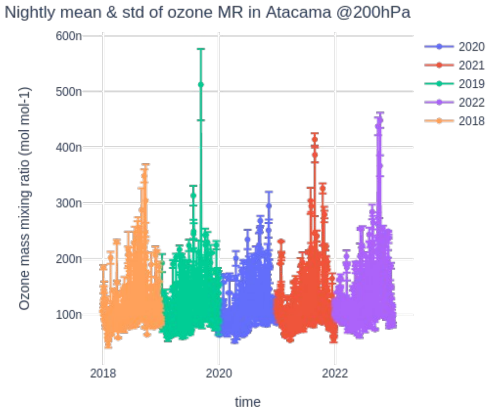

Nightly mean & std of ozone MR in Atacama @650hPa

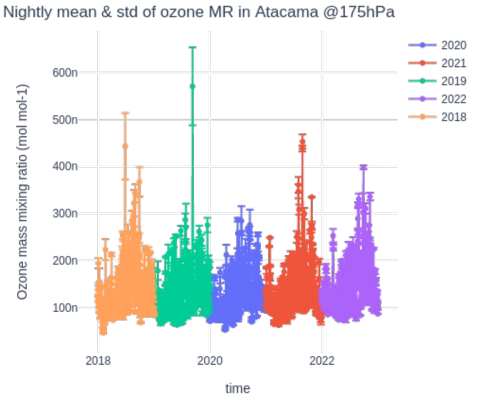

Nightly mean & std of ozone MR in Atacama @ 600hPa

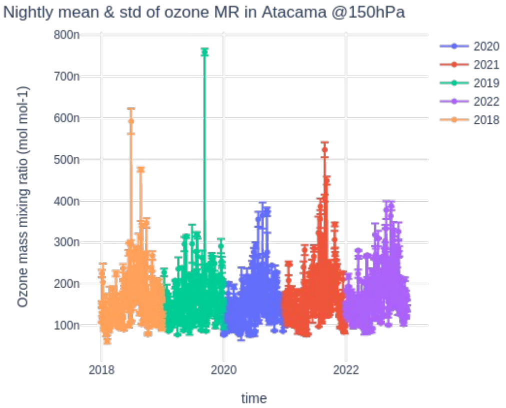

Nightly mean & std of ozone MR in Atacama @ 500hPa

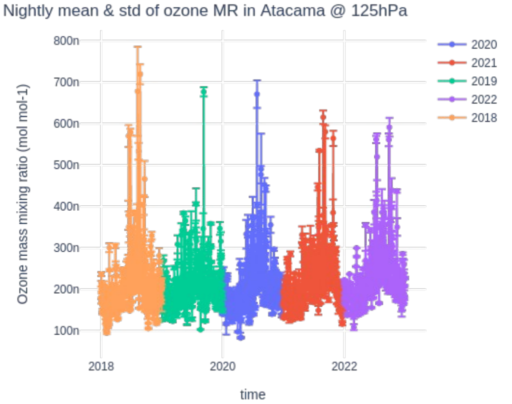

Nightly mean & std of ozone MR in Atacama @ 250hPa

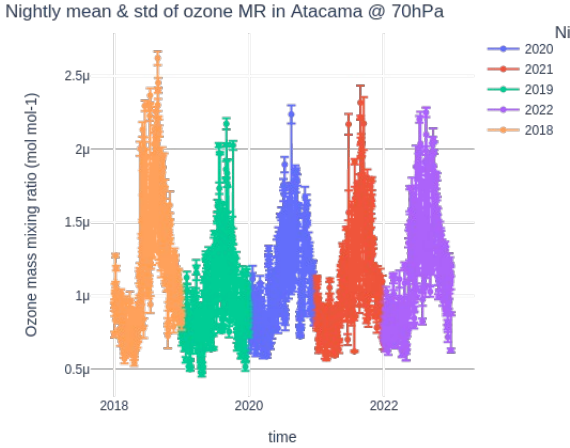
Ozone mixing ratios per pressure level (South)

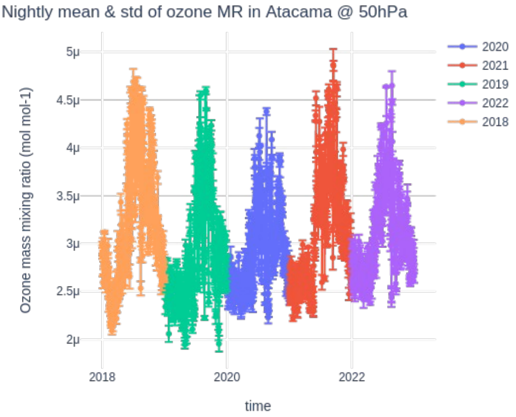

Nightly mean & std of ozone MR in Atacama @200hPa

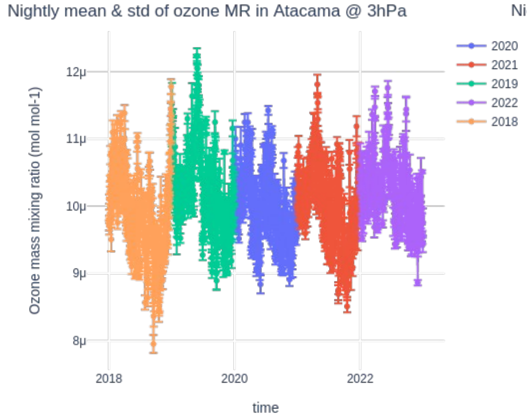

Nightly mean & std of ozone MR in Atacama @175hPa

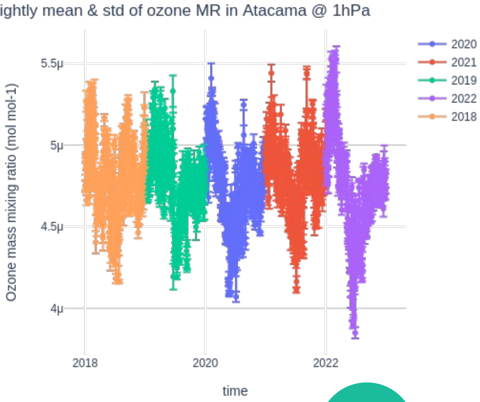

Nightly mean & std of ozone MR in Atacama @150hPa


Nightly mean & std of ozone MR in Atacama @ 125hPa


Nightly mean & std of ozone MR in Atacama @ 70hPa


Nightly mean & std of ozone MR in Atacama @ 50hPa


Nightly mean & std of ozone MR in Atacama @ 3hPa


Nightly mean & std of ozone MR in Atacama @ 1hPa

Production of ozone absorption profile

Ozone absorption per wavelength per height bin, in a format compatible with the CTAO simulation tools (sim_telarray)

1) **ozone_MR** (mol/mol) * **atmospheric_density** (g/cm^3) * **N_A** (particle x mol^{-1}) / **MolarMassOzone** (kg.mol)) → **ozone number density (**particle/m^3**)**

2) **a(H, λ) = ozone number density (**particle/m^3**) * Cross section (**m^2/particle**)**

   The cross section was retrieved from V. Gorshelev et al, AMT, 7, 609–624, 2014

3) **Integrate a(λ)** for various altitudes in order to obtain optical depth (OD)

We have all we need to run simulations in order to estimate the effect of ozone

- ➢ As a first approximation we will use the testeff program, provided as a part of the sim_telarray package

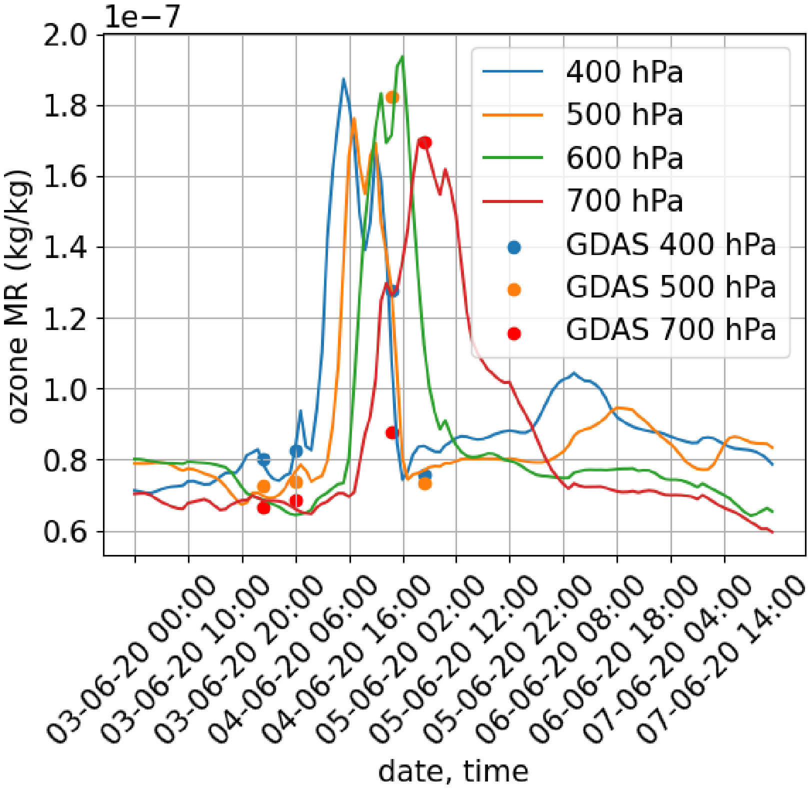
Extreme events

Transport of ozone masses from the Stratosphere to the Troposphere (STT)

- STT example happened 4th - 5th of June 2020, over the South site
- ~ 2 days duration, ozone seems to reside few hours to each pressure level
- Recorded both by GDAS & ECMWF

On going studies

- Effect of STT events on the light density on the ground & the IRFs
- How frequently such events are occuring?
- Correlations with other phenomena?



Seasonal variations and extreme events

Example: preliminary results, only ozone extinction, comparison between a day in June and a day in May

- Differences within 1-2% have been observed
- A conclusive study on the need for ozone calibration requires the comparison in (energy bias, effective area) between an average ozone profile and various extreme (but natural) ozone profiles
- Decide whether to disentangle (or not) from Rayleigh Scattering and average aerosol extinction profiles for each site

λ range	Zd	Emission alt	Optical efficiency (05/25/2020 / 05/06/2020)
nm	deg	Km (a.s.l.)	%
290 – 750	0	12.585	98.3

Nitrogen oxides

NO_x molecules also absorb in the spectrum range of interest

We focus on NO_2

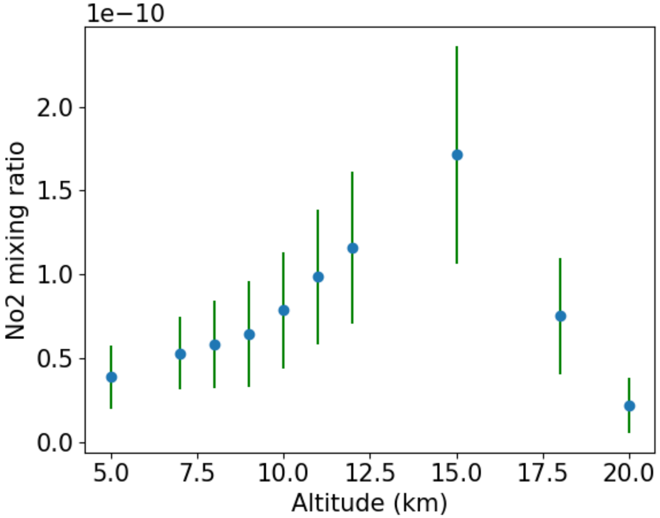
- Larger mixing ratio wrt NO
- Absorption cross section available in HITRAN

Analysis of 4 months of data over La Palma (Sep-Dec 2023)

- Copernicus Atmospheric Monitoring Service (CAMS) global reanalysis (EAC4)

Motivations for the study

- Time variability of NO_2 mixing ratio
  - Lightnings, pollution from aircrafts
- Light density on the ground, with/without NO_2 absorption
  - Definition of calibration strategy



λ range	Zd	Emission altitude (a.s.l.)	Optical efficiency (with NO_2 / without)
290 – 750 (nm)	0 deg	9.851 km	99.99 %
290 – 750 (nm)	0 deg	12.585 km	99.98 %

Conclusion

The first version of the molecular atmosphere calibration has been developed

Calibration software that assess the effect of absorbing molecules has been developed

- Preliminary results of their impact and their variations are presented here

Next Steps

- **Shower development & light creation**
  1) Revisit uncertainty budget estimation for the CTAO north site using ERA-5 datasets; studies for the south site are in planning.
  2) Validation of DAS datasets with dedicated radiosonde campaigns & surface data from weather stations
  3) Discuss an approach to estimate the systematic uncertainty budget for tailored simulations
- **Molecular extinction**
  1) Include temperature dependence of absorption cross sections.
  2) Conduct simulations to refine systematic uncertainty budget and define a detailed calibration strategy.