DEAP algorithm for the retrieval of aerosol extinction and NO_2 vertical profiles over the Po Valley

P. Pettinari[1], E. Castelli[1], E. Papandrea[1], M. Valeri[2], F. Hendrick[3], C. Fayt[3], S. Beirle[4], M. M. Friedrich[3], M. Van Roozendael[3]

[1] CNR-ISAC, Bologna (Italy)
[2] SERCO Italia S.p.A., Frascati
[3] BIRA-IASB, Belgium
[4] MPIC, Mainz

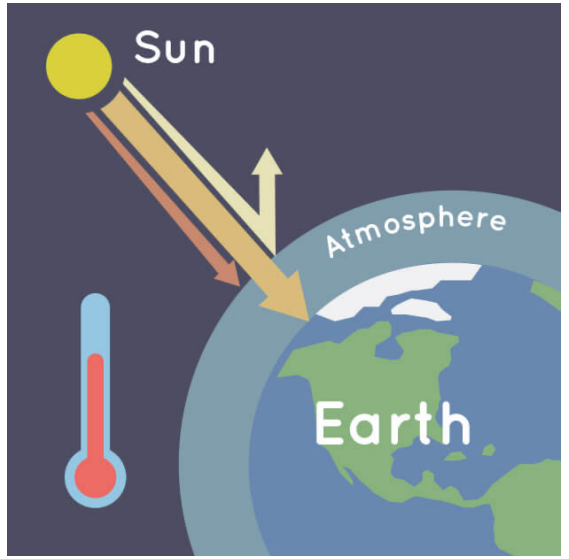
RAMI workshop, Varese (Italy), 8 June 2023

Why NO_2 measurements?

SOURCES
Combustion processes:
- Traffic
- Factories

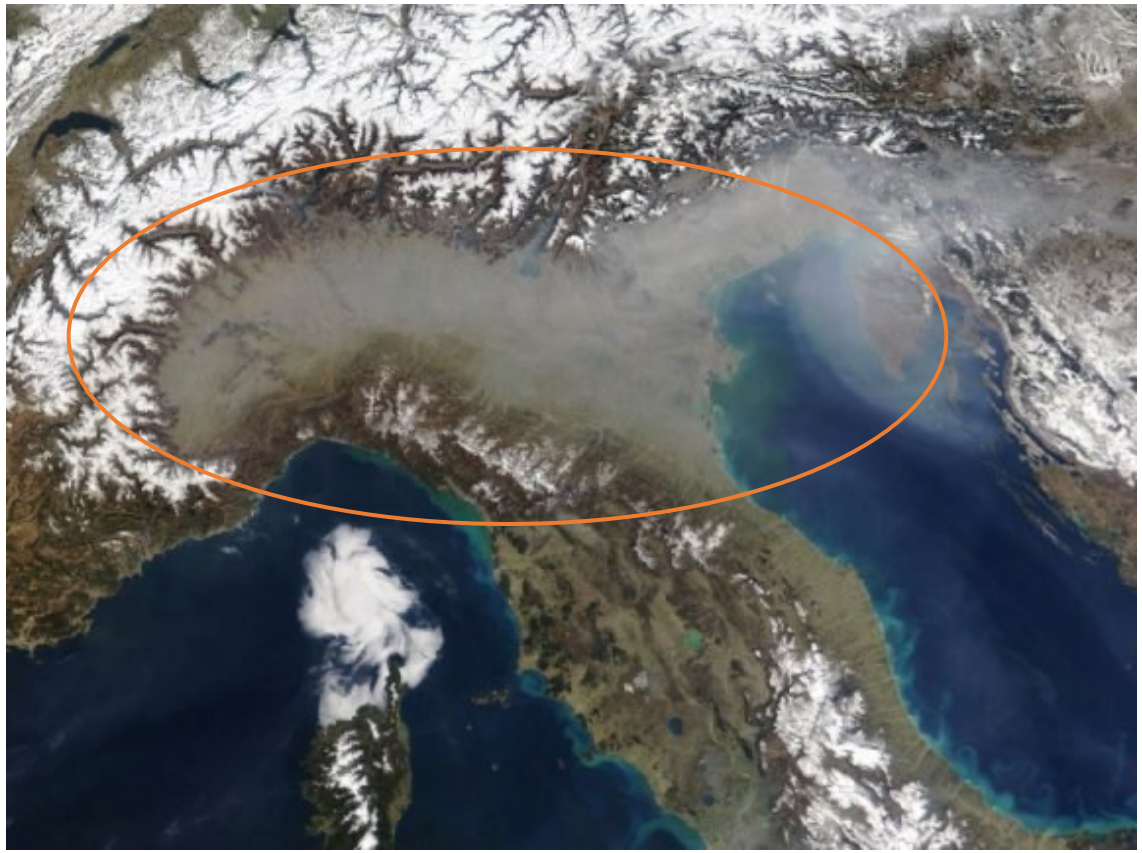
RISKS
- Intensify responses to allergens
- Premature death
- Cardiopulmonary effects
- Respiratory symptoms

OTHER EFFECTS
Tropospheric O_3 formation:
- Respiratory symptoms
- Greenhouse effect



esa IDEAS-QA4EO CNR ISAC DOAS-BO

Why especially in the Po Valley?

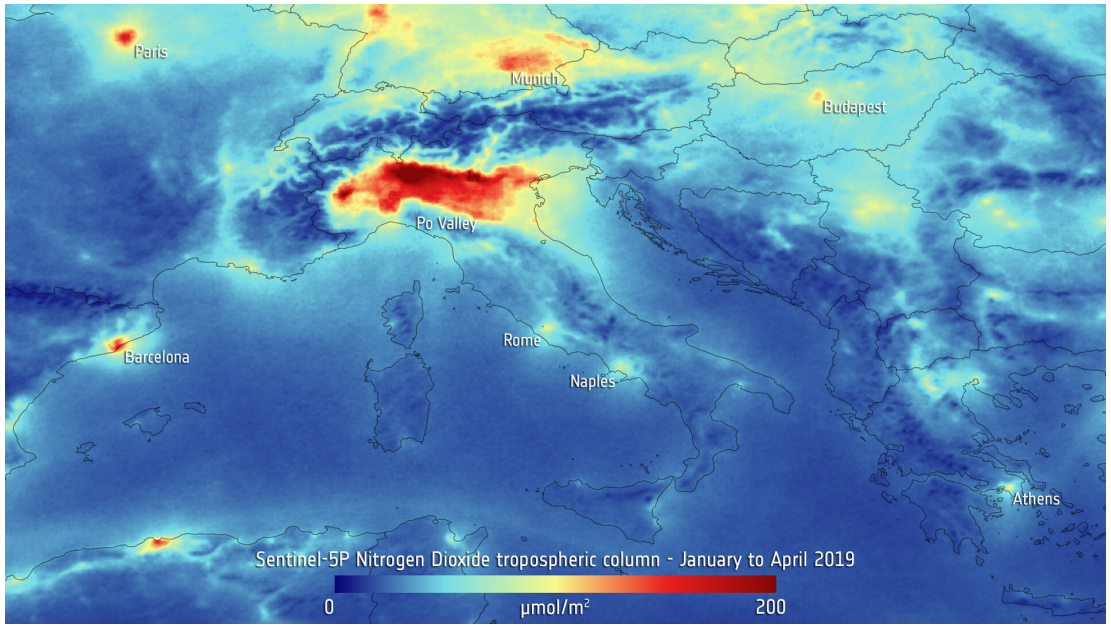


- One of the most polluted regions in Europe.
- The most industrialized area in Italy.
- Geography prevents air mixing. The valley is closed between the mountains.
- Major problems in winter when thermal inversions and foggy days occur.

esa IDEAS-QA4EO CNR ISAC DOAS-BO

Most common NO_2 measurement methods

SATELLITE REMOTE SENSING



- Columnar concentrations
- Global coverage
- Low spatial and temporal resolution

IN-SITU

- High temporal resolution
- High accuracy
- Poor vertical and horizontal coverage

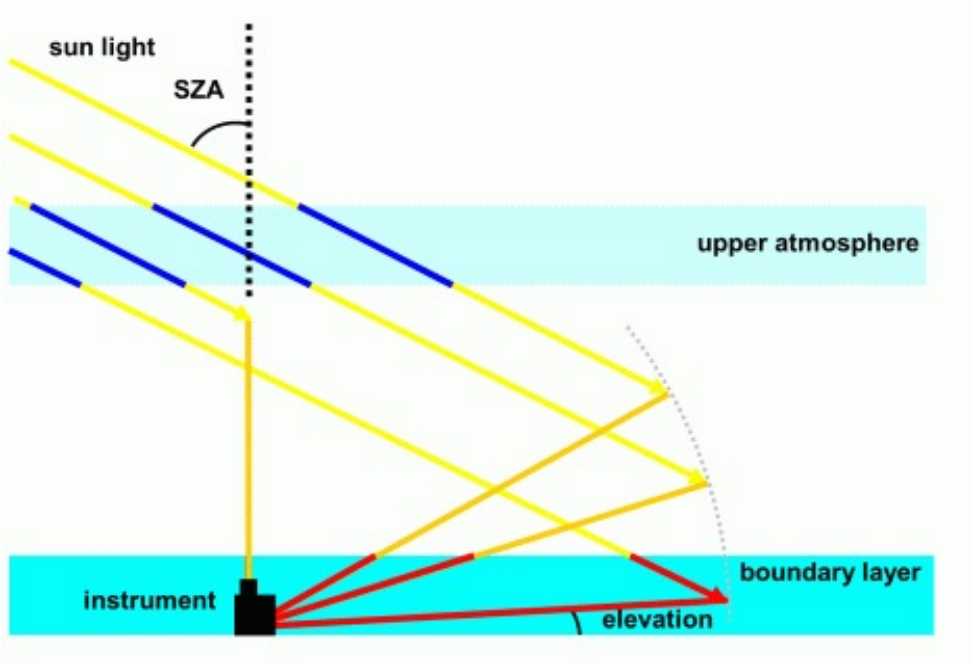
esa

IDEAS-QA4EO

CNR ISAC

DOAS-BO

Multi Axis (MAX)-DOAS measurements



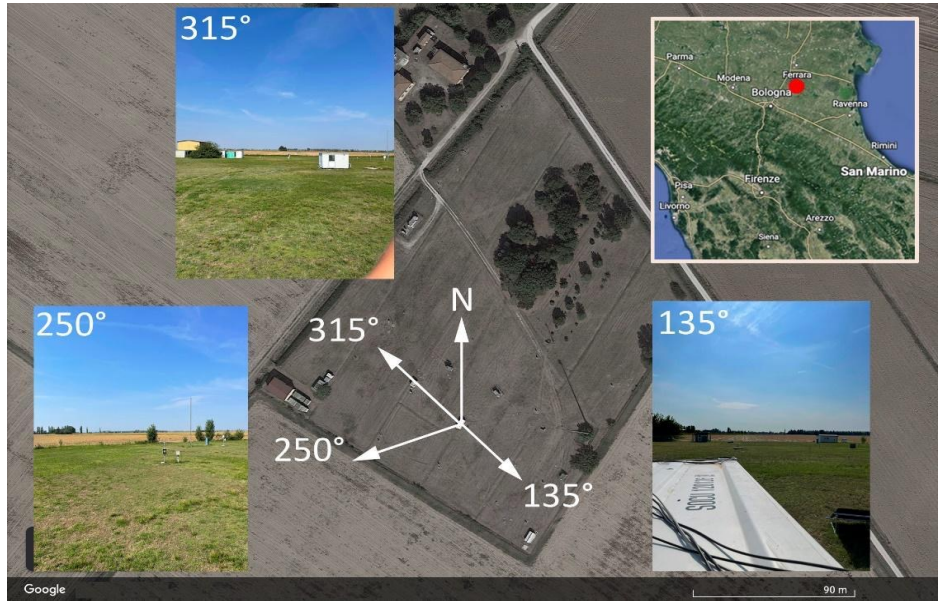
For each scan, several spectra (VIS and UV) at different elevation angles are measured.

One vertical profile, of an absorbing gas, can be retrieved for each scan.

- **Measurments sensitive to the lower troposphere (from 0 to 4 km).**
- **Information resolved along the vertical direction.**
- **Possibility to measure at different azimuth directions.**
- **High temporal resolution and sampling (about 2 minutes per scan).**

esa IDEAS-QA4EO CNR ISAC DOAS-BO

SkySpec-2D instrument in the Po Valley



WHAT DOES IT MEASURE?	MAX-DOAS scans
AZIMUTH DIRECTIONS	135°, 250°, 315°
ELEVATION ANGLES	1°, 2°, 3°, 5°, 10°, 30°, 90°
SPECTRAL BANDS	**VIS (410-550 nm)** UV (305-405 nm)
SPECTRAL RESOLUTION	0.6 nm

(Pettinari et al. 2022, Towards a new MAX-DOAS measurement site in the Po Valley: NO_2 total VCDs)

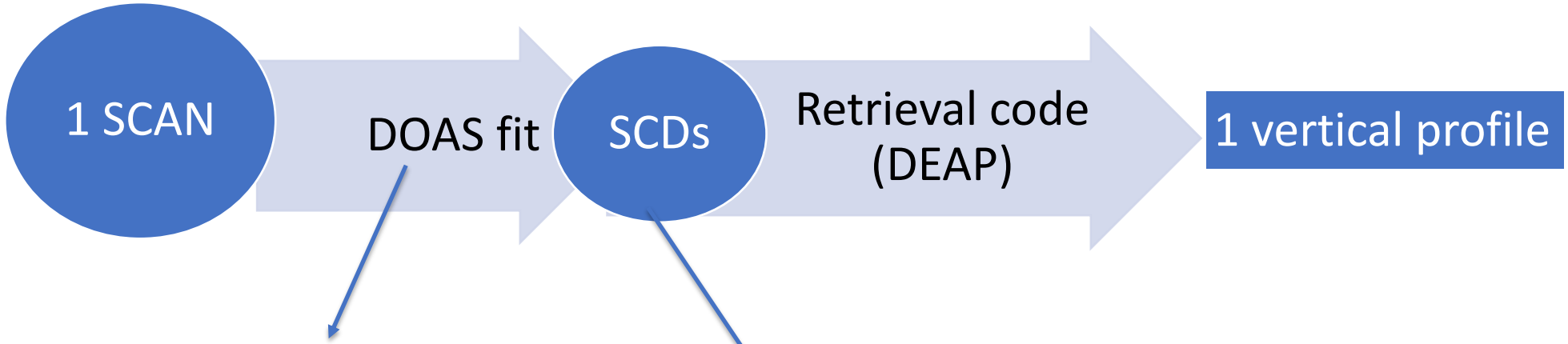
esa

CNR ISAC

DOAS-BO

IDEAS-QA4EO

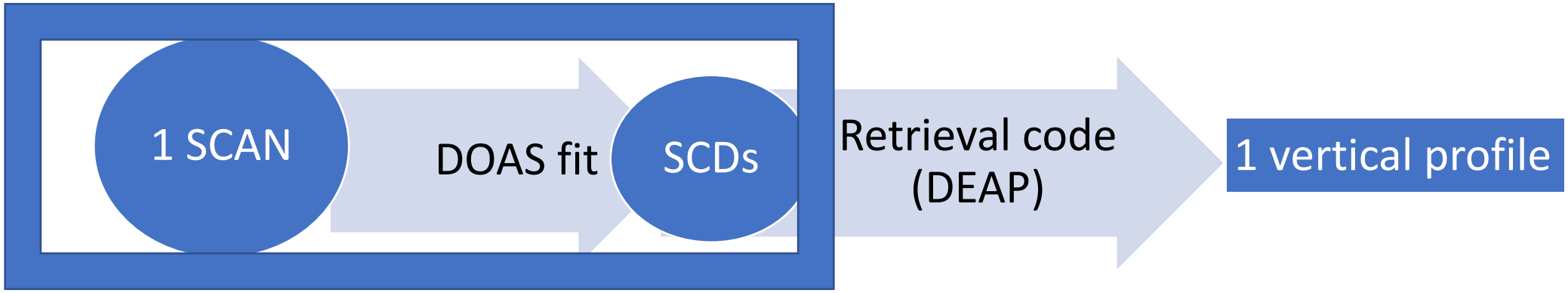
Retrieval method



Differential Optical Absorption Spectroscopy technique

Slant Column Densities (SCDs) are gas concentrations integrated along the slant path crossed by the light in atmosphere.

Retrieval method: DOAS fit



SCD of jth gas

Measured spectrum

$$ln\left(\frac{I^*(\lambda, L)}{I_0'^*(\lambda, L)}\right) \approx \sum_j \bar{c}_j L ln\left[\int_{-\Delta\lambda}^{\Delta\lambda} e^{-\sigma'(\lambda-\lambda')} H(\lambda')d\lambda'\right]$$

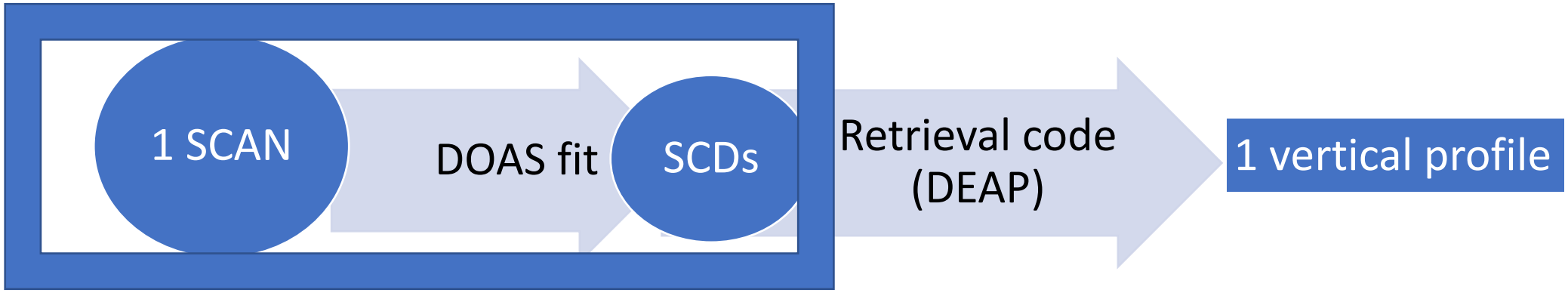
Reference spectrum

Absorption cross section

Instrumental function

esa IDEAS-QA4EO CNR ISAC DOAS-BO

Retrieval method: DOAS fit



SCD of jth gas

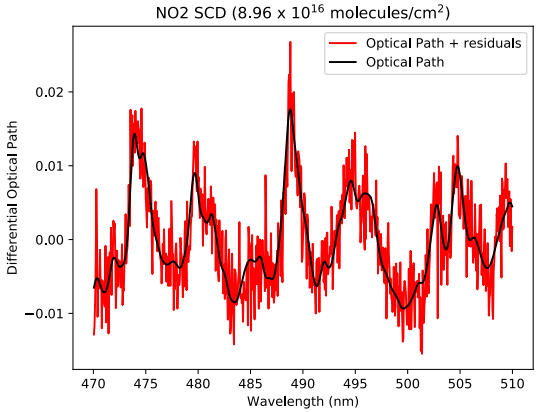
Measured spectrum

$$ln\left(\frac{I^*(\lambda, L)}{I_0'^*(\lambda, L)}\right) \approx \sum_j \bar{c}_j L ln\left[\int_{-\Delta\lambda}^{\Delta\lambda} e^{-\sigma'(\lambda-\lambda')} H(\lambda')d\lambda'\right]$$

Reference spectrum

Absorption cross section

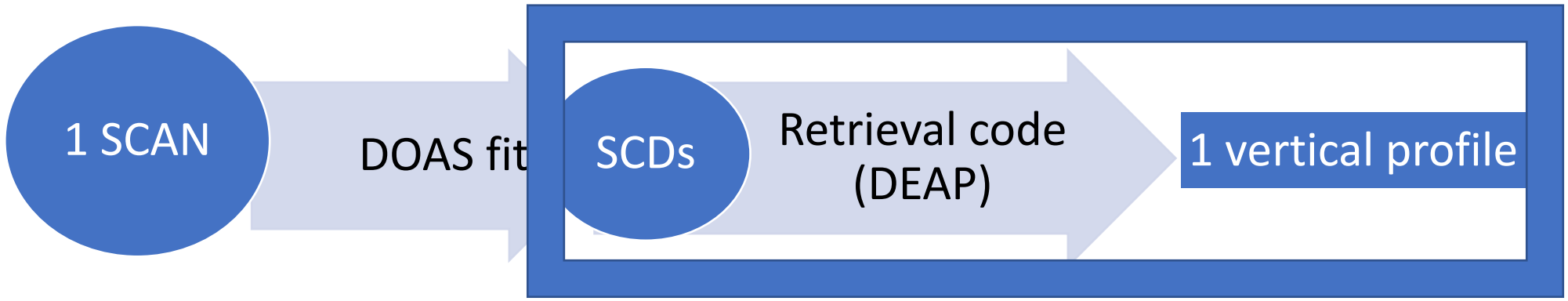
Instrumental function



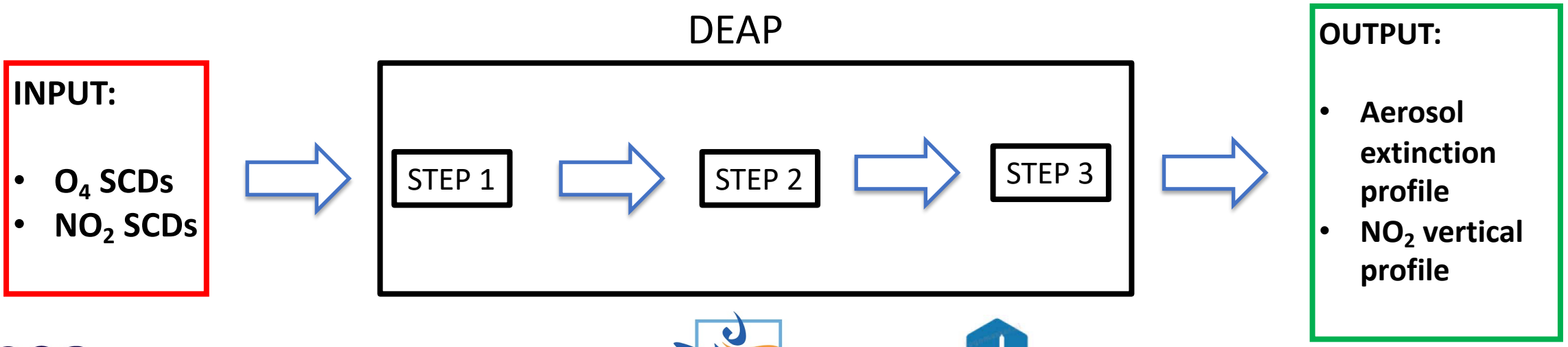
This part is no time-consuming (order of seconds!!)

esa IDEAS-QA4EO CNR ISAC DOAS-BO

Retrieval method: DEAP retrieval

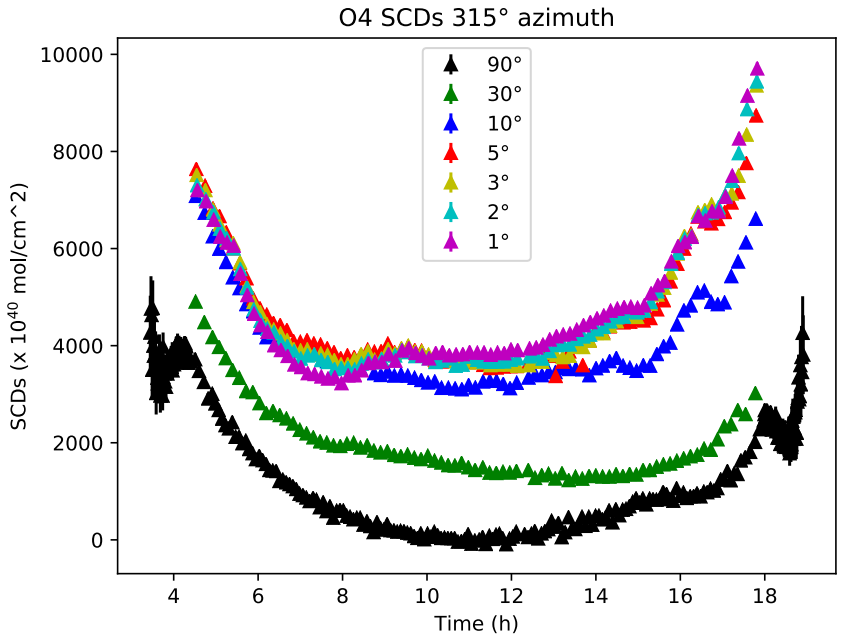


The DEAP (DOAS optimal Estimation Atmospheric Profile retrieval) code is an Optimal Estimation algorithm that exploits the SCIATRAN code (Rozanov et al. 2014) as forward model. Time-consuming part (about 15 min. per profile!!).



esa IDEAS-QA4EO CNR ISAC DOAS-BO

DEAP retrieval: step 1 (retrieval of aerosol extinction profile from O_4 SCDs)

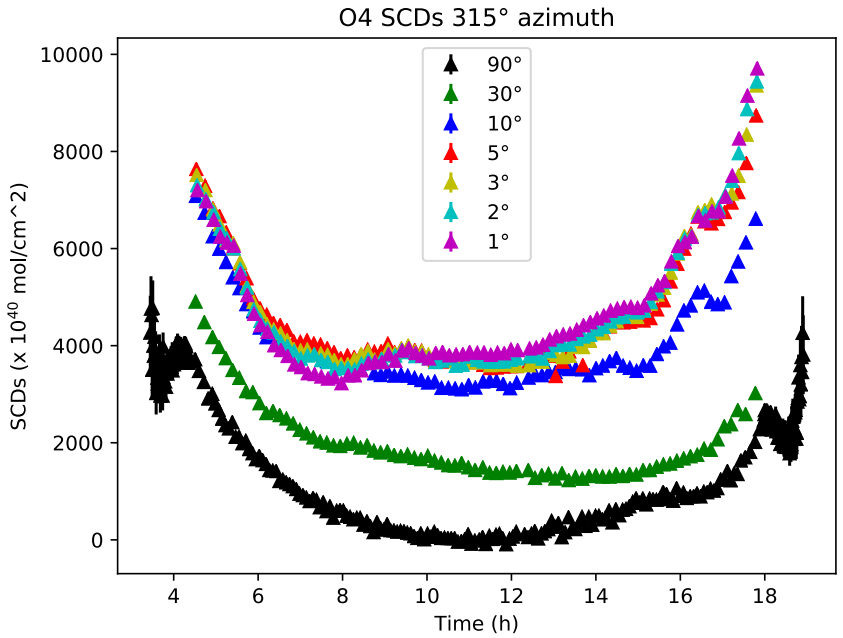


Why O_4 SCDs for aerosol?

$$x_{i+1} = x_i + (K^T S_y^{-1} K + S_0^{-1} + g K^T S_y^{-1} K)^{-1} (K^T S_y^{-1}(y - y_i) - S_0^{-1}(x_i - x_0))$$

y=O_4 SCD
K=d O_4 SCD/ d aer_ext
x =aer_ext

DEAP retrieval: step 1 (retrieval of aerosol extinction profile from O_4 SCDs)



Why O_4 SCDs for aerosol?

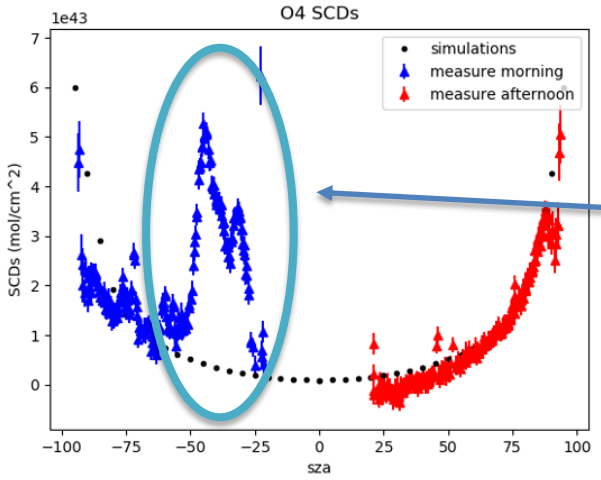
Clouds and aerosol affect the O_4 SCDs

O_4 SCD $\propto$ Atmospheric path

O_4 SCD $\propto$ ~~Atmospheric concentration~~

$$x_{i+1} = x_i + (K^T S_y^{-1} K + S_0^{-1} + g K^T S_y^{-1} K)^{-1} (K^T S_y^{-1}(y - y_i) - S_0^{-1}(x_i - x_0))$$

y=O_4 SCD
K=d O_4 SCD/ d aer_ext
x =aer_ext



Assumption: constant O_4 distribution in time and space.

Effect of clouds

DOAS-BO

IDEAS-QA4EO

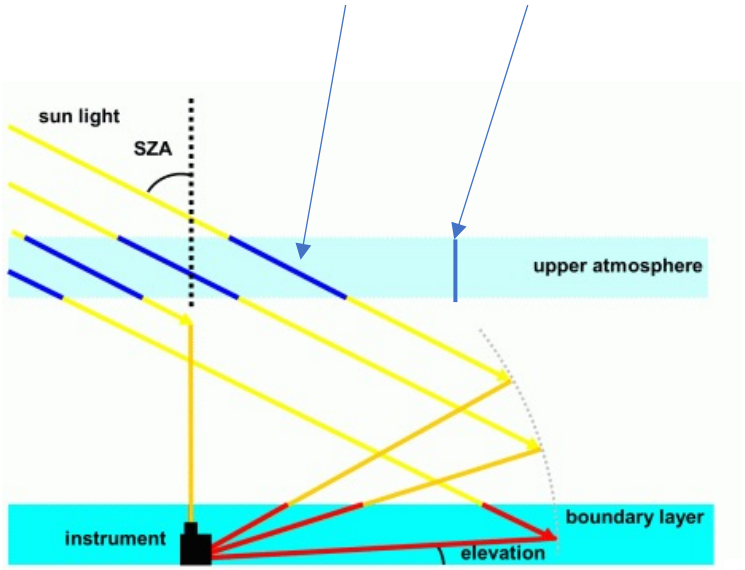
esa

CNR ISAC

DEAP retrieval: step 2 (Box-AMFs simulation)

What are box-AMFs (Air Mass Factors)?

- Defined for each retrieval layer
- Depend on scattering processes (aerosol content, surface albedo …)
- Ratio between SCD and VCD



How simulate them?

- SCIATRAN code that accounts for scattering processes
- Aerosol extinction profile retrieved in step 1 used as input for simulation

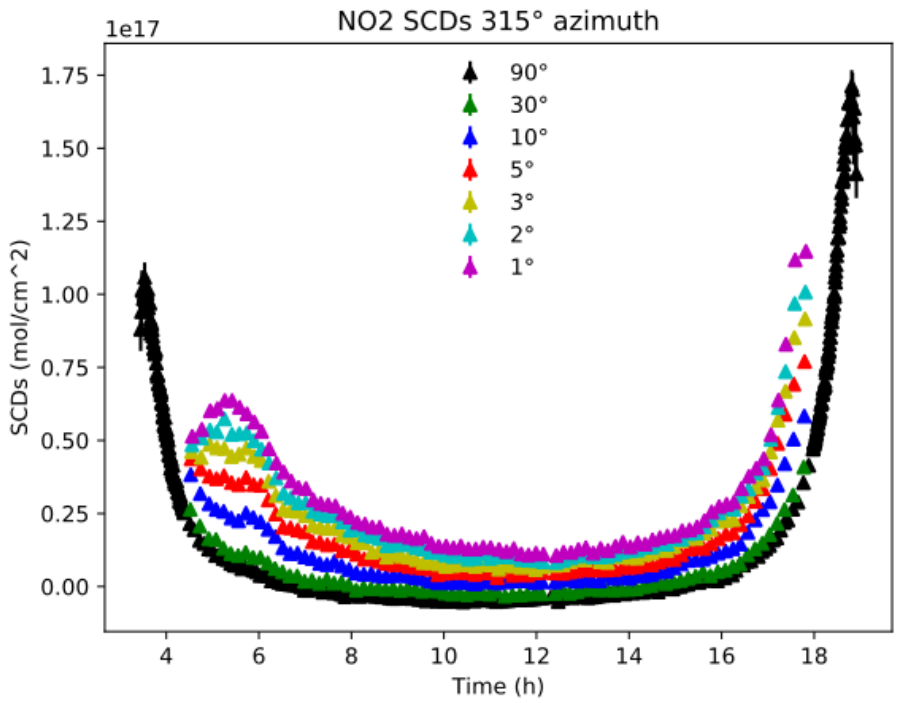
Why simulate them?

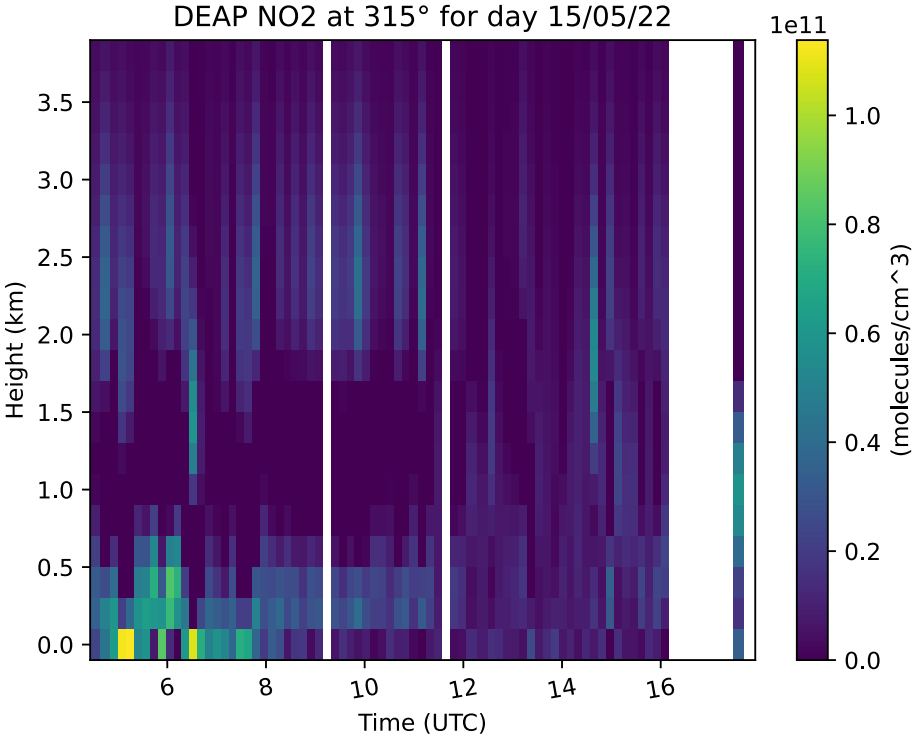
- Important for the step 3:

NO_2 SCD $\propto$ Atmospheric path (known!)

NO_2 SCD $\propto$ Atmospheric NO_2 concentration

DEAP retrieval: step 3 (retrieval of NO_2 vertical profile from NO_2 SCDs and box-AMFs)

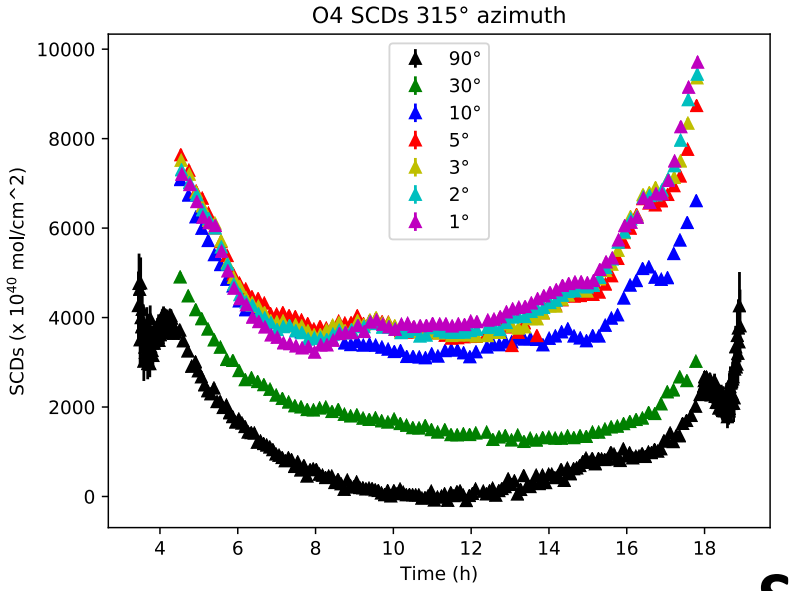




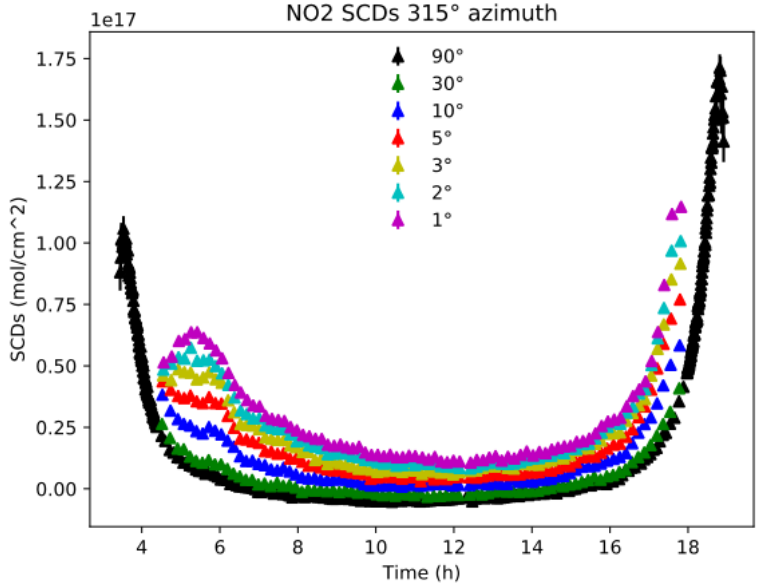
$$x_i = x_0 + S_0 K^T (K S_0 + S_0 K^T + g S_y)^{-1} (y - K x_0)$$

y=NO_2 SCD
K=NO_2 box-AMF
x =NO_2_conc

DEAP retrieval: summary

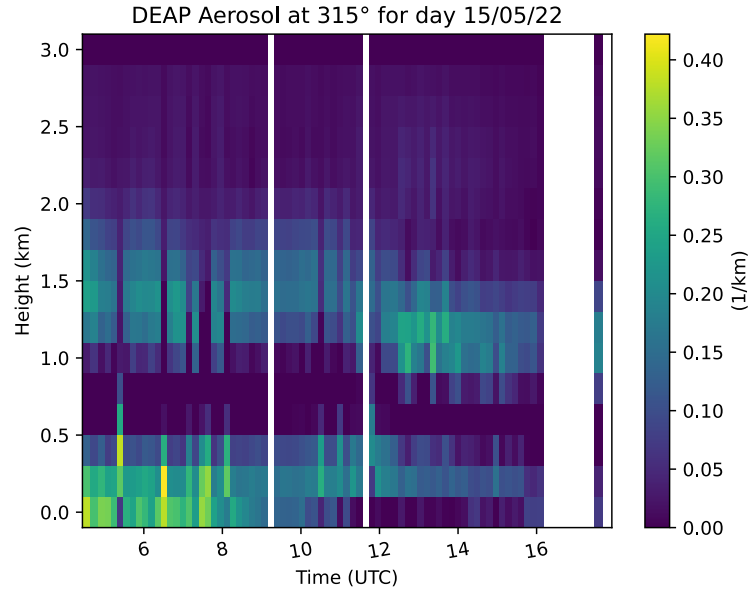


SCDs

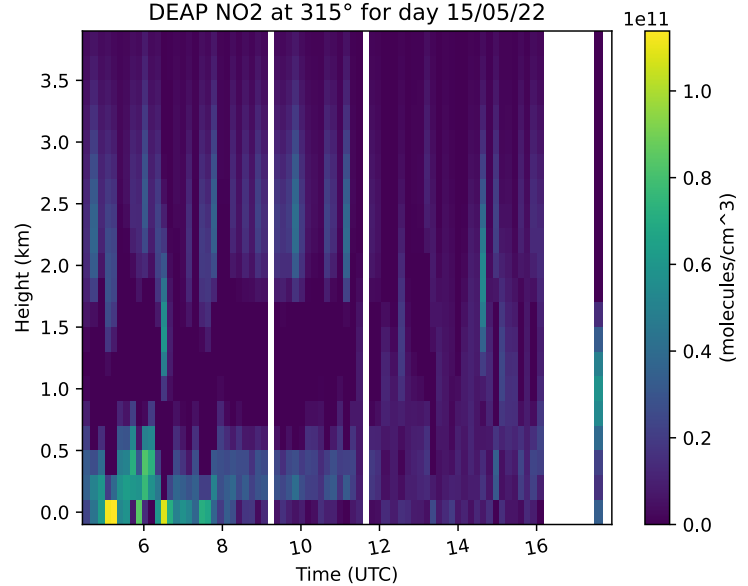


DEAP retrieval algorithm

Aerosol Extinction



NO_2



esa

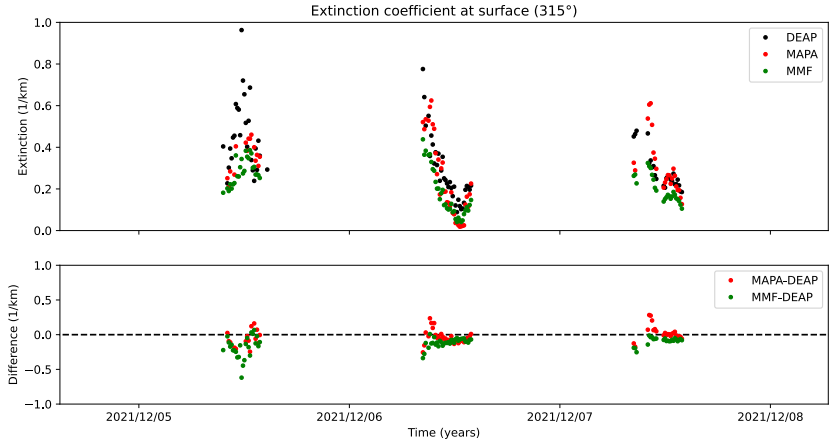
DOAS-BO

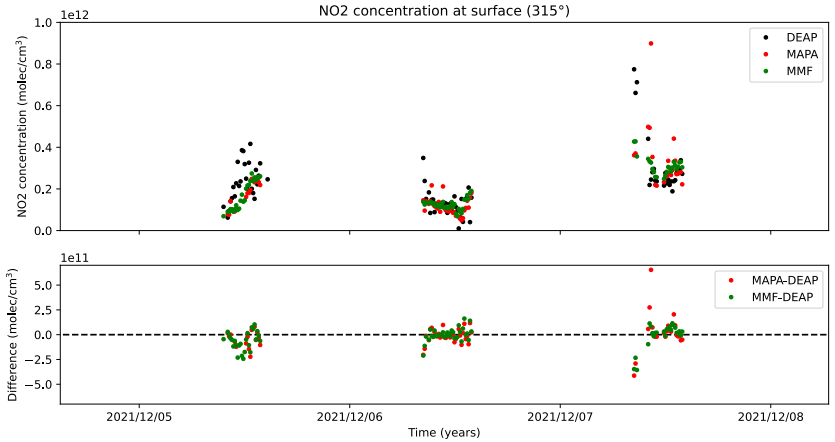
IDEAS-QA4EO

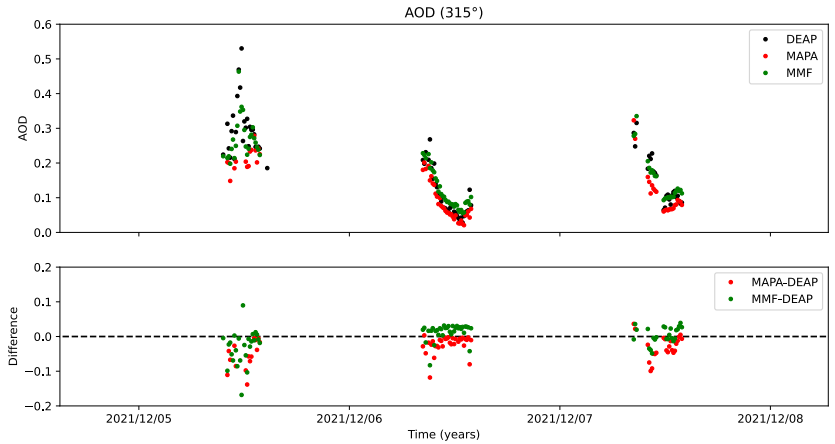
CNR ISAC

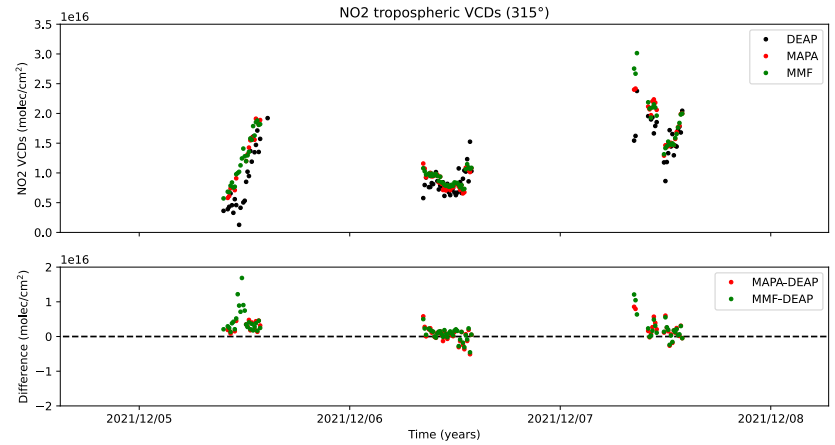
Comparison with MMF and MAPA (315° azimuth)

MMF and MAPA are the reference retrieval algorithms used for the Fiducial Reference Measurements for DOAS (FRM4DOAS) centralized processing.









Results from 1 October 2021 to 23 March 2022

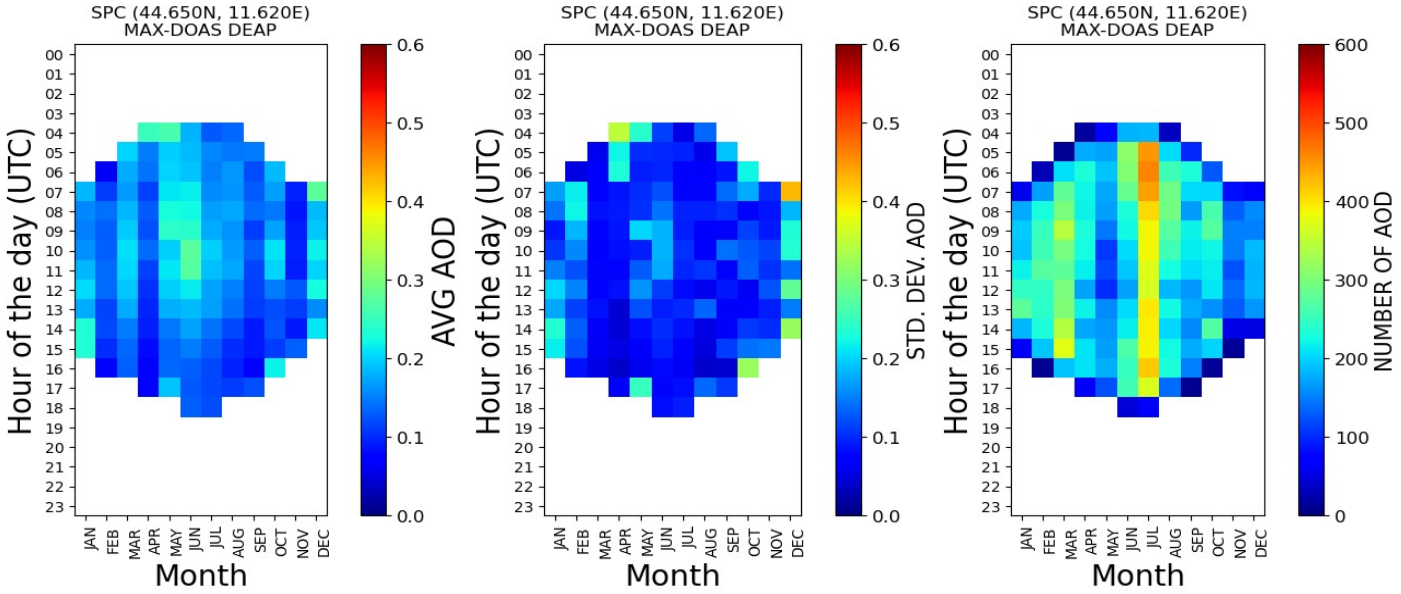
		MAPA vs DEAP	MMF vs DEAP
EXT SURF	CORR	0.79	0.82
	BIAS (1/km)	-0.025	-0.08
AOD	CORR	0.54	0.94
	BIAS	0.025	0.007
NO_2 SURF	CORR	0.61	0.73
	BIAS ($x10^{10}$ molec/cm^3)	4.2	2.1
NO_2 VCDs	CORR	0.71	0.56
	BIAS ($x10^{15}$ molec/cm^2)	1.3	2.2

CNR ISAC esa IDEAS-QA4EO DOAS-BO

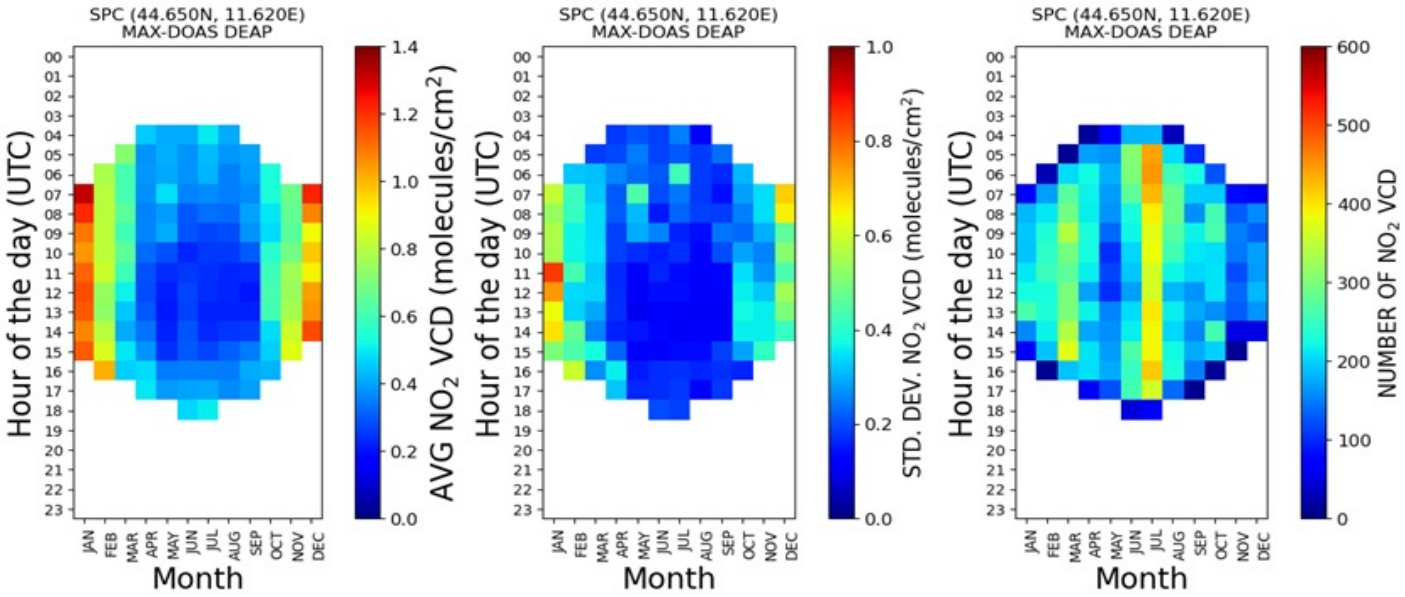
Tropospheric AOD and NO_2 VCDs in the Po Valley

- Vertical profiles used to compute integrated tropospheric quantities (AOD and NO_2 VCDs)
- The whole dataset goes from 1 October 2021 to now.
- Here, we show 1 year of data (from 1 October 2021 to 31 September 2022)
- All data in the three azimuth directions averaged.

AOD



NO_2 VCDs (x10^{16})



(project report: Valeri M. et al., Report on the intercomparison results between ground-based and satellite measurements)

IDEAS-QA4EO

DOAS-BO

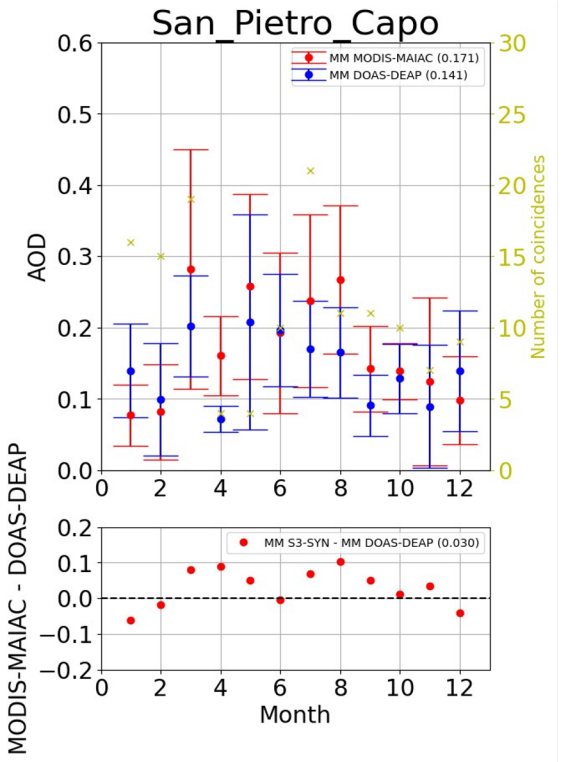
esa

CNR ISAC

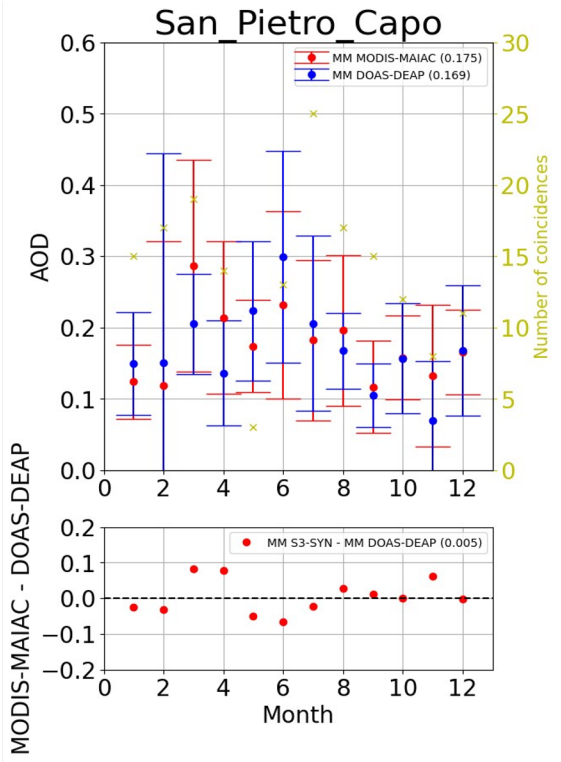
Comparison with satellite data (MODIS): AOD (0.47 μm)

1 year of data – all three directions - MODIS data within a 5x5 km^2 pixel around station are averaged – MAX-DOAS data within ± 30 min. around MODIS overpass are averaged

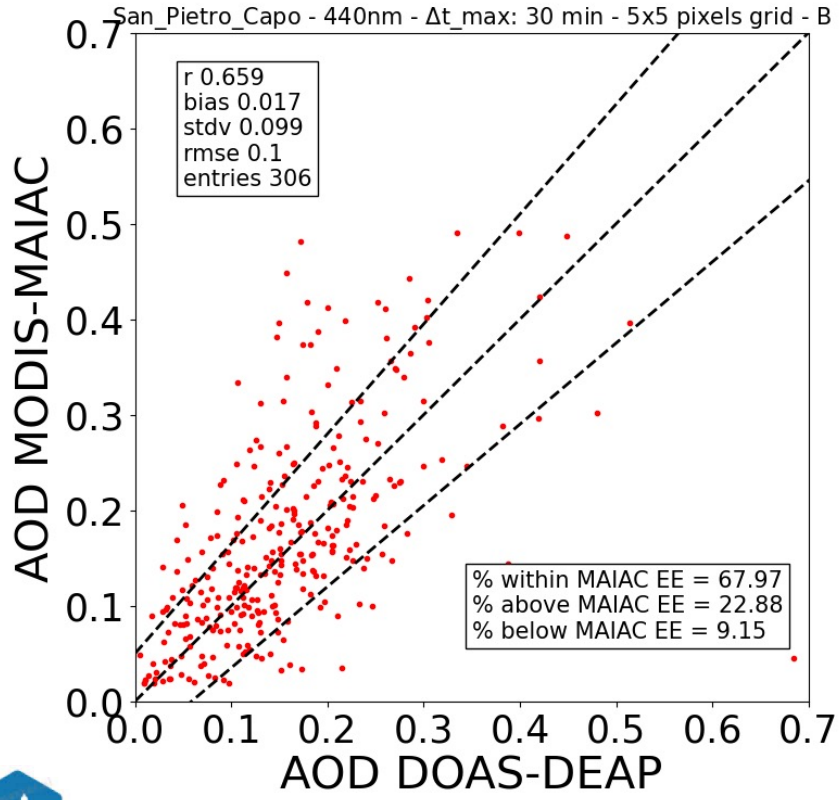
MODIS/Aqua



MODIS/Terra



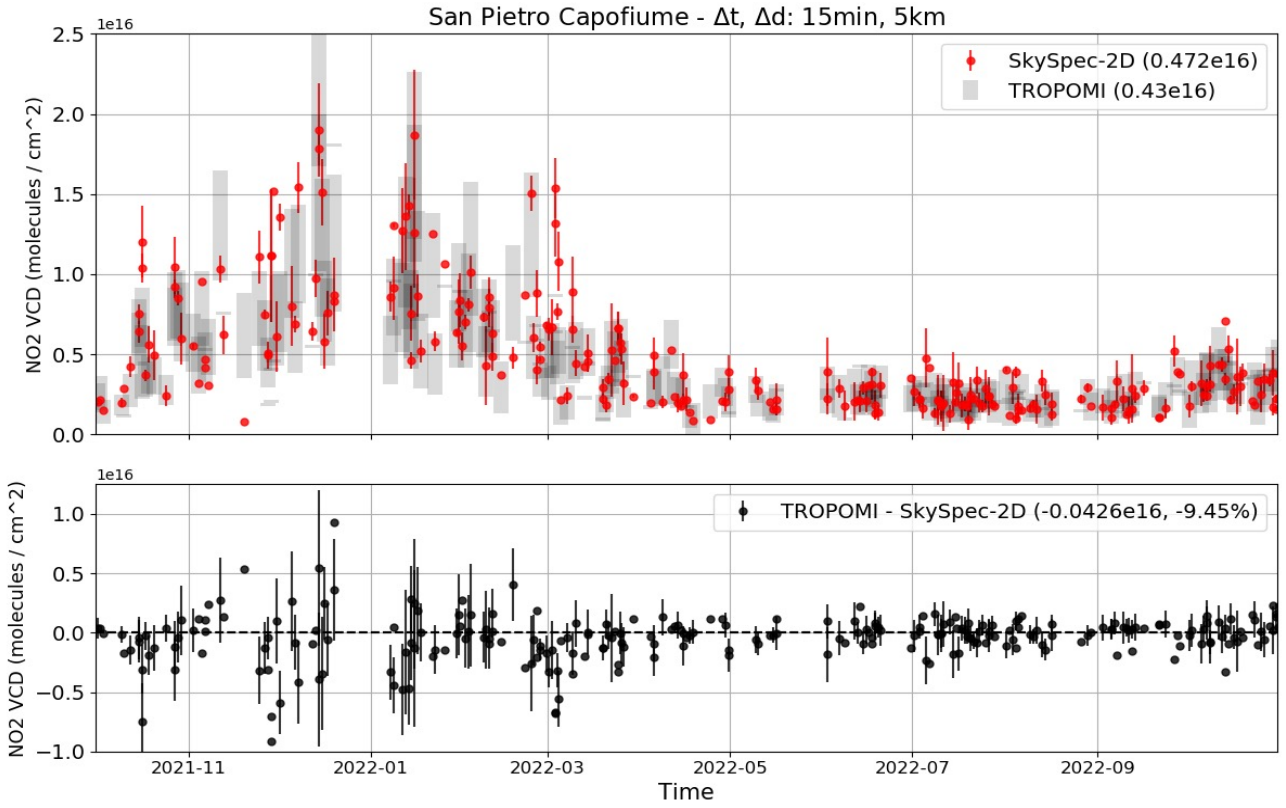
MODIS/ Aqua + Terra

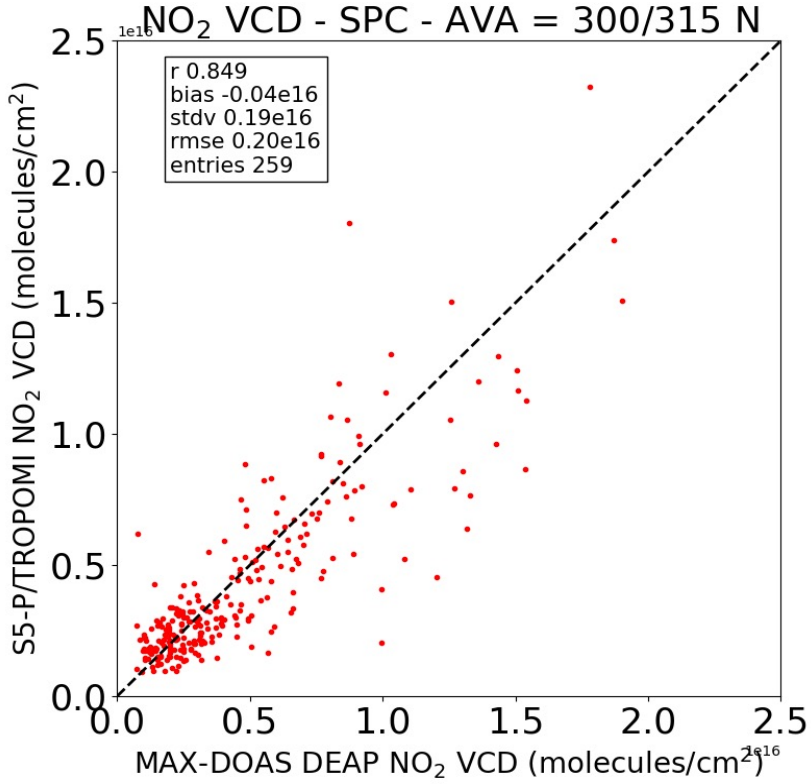


esa IDEAS-QA4EO CNR ISAC DOAS-BO

Comparison with satellite data (Tropomi): NO_2 VCDs

1 year of data - only direction at 315° - TROPOMI data within a radius of 5 km around station are averaged – MAX-DOAS data within ± 15 min. around Tropomi overpass are averaged





esa IDEAS-QA4EO CNR ISAC DOAS-BO

ITINERIS project for the future

The Italian Integrated Environmental Research Infrastructures Systems (ITINERIS) is a project coordinated by the Consiglio Nazionale delle Ricerche (CNR) with the purpose to build an Italian hub of research infrastructures in the environmental scientific domain.

A new Fourier Transform Infra-Red (FTIR) spectrometer will be acquired in the next future.

- Infra-red spectra measured with a high spectral resolution compliant to NDACC
- Useful to measure many other trace gases present over the Po Valley.

Spectral resolution	0.0063 cm^{-1}
Spectral range	800 - 14,000 cm^{-1}

ITINERIS

CNR ISAC

Conclusions

- DEAP algorithm is used to retrieve aerosol extinction and NO_2 vertical profiles from MAX-DOAS scans (about 15 min. per scan).
- At the moment, DEAP retrieved data over the Po Valley from 1 October 2021 till now.
- DEAP in good agreement with the reference algorithms MAPA and MMF.
- Good agreement between DEAP and TROPOMI NO_2 tropospheric VCDs (corr=0.85). TROPOMI underestimates the NO_2 of about 10%.
- Good agreement between DEAP and MODIS AOD (corr=0.66). DEAP has a negative bias of about 0.03 (MODIS/Aqua) and 0.005 (MODIS/Terra).
- Recently, DEAP was also exploited to retrieve NO_2 and extinction vertical profiles from MAX-DOAS scans acquired in Tor Vergata (Rome).

FUTURE DEVELOPMENTS:

- Improve the DEAP algorithm (speed, convergence)
- Exploit DEAP to retrieve Formaldehyde (HCHO) in the Po Valley
- Measurement of new species over the Po Valley (ITINERIS project)

ITINERIS esa IDEAS-QA4EO CNR ISAC DOAS-BO