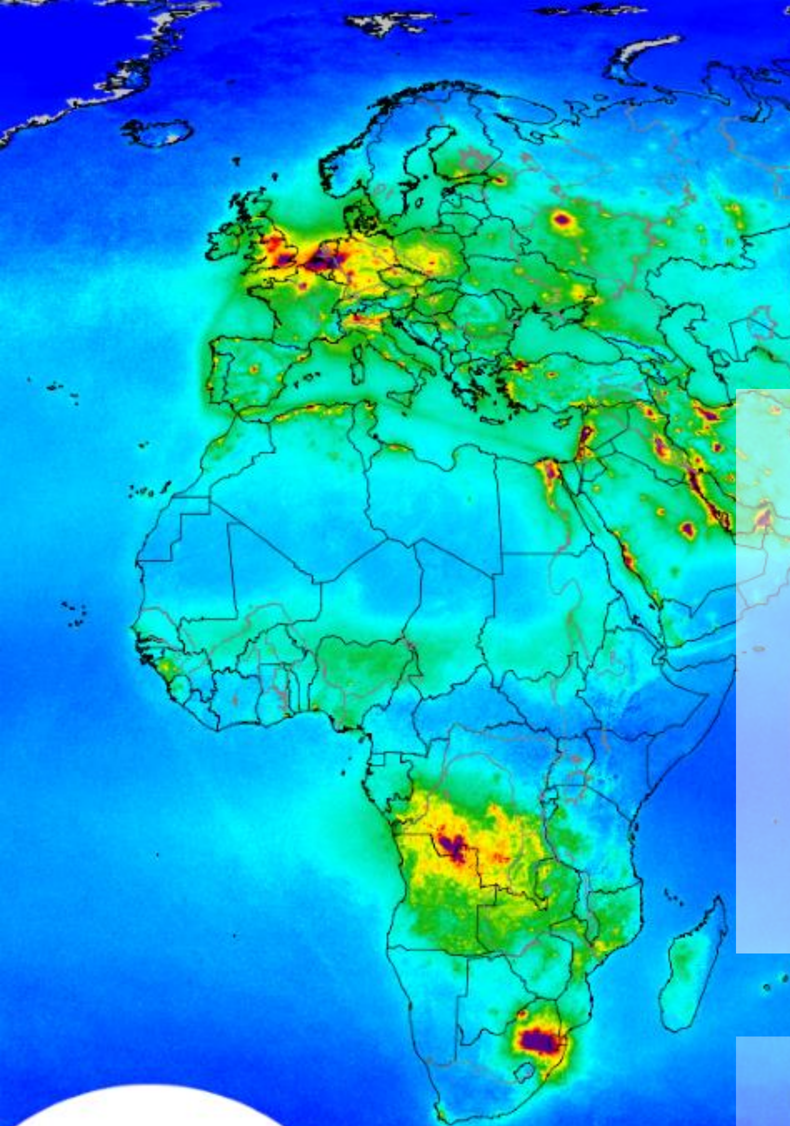

Satellite retrievals of aerosols and trace gases

Anu-Maija Sundström
Finnish Meteorological Institute

Fourth Joint School on Atmospheric Composition

28 Sept – 6 October 2022

Copernicus Europe's eyes on Earth
ECMWF
Atmosphere Monitoring Service atmosphere.copernicus.eu
EUMETSAT
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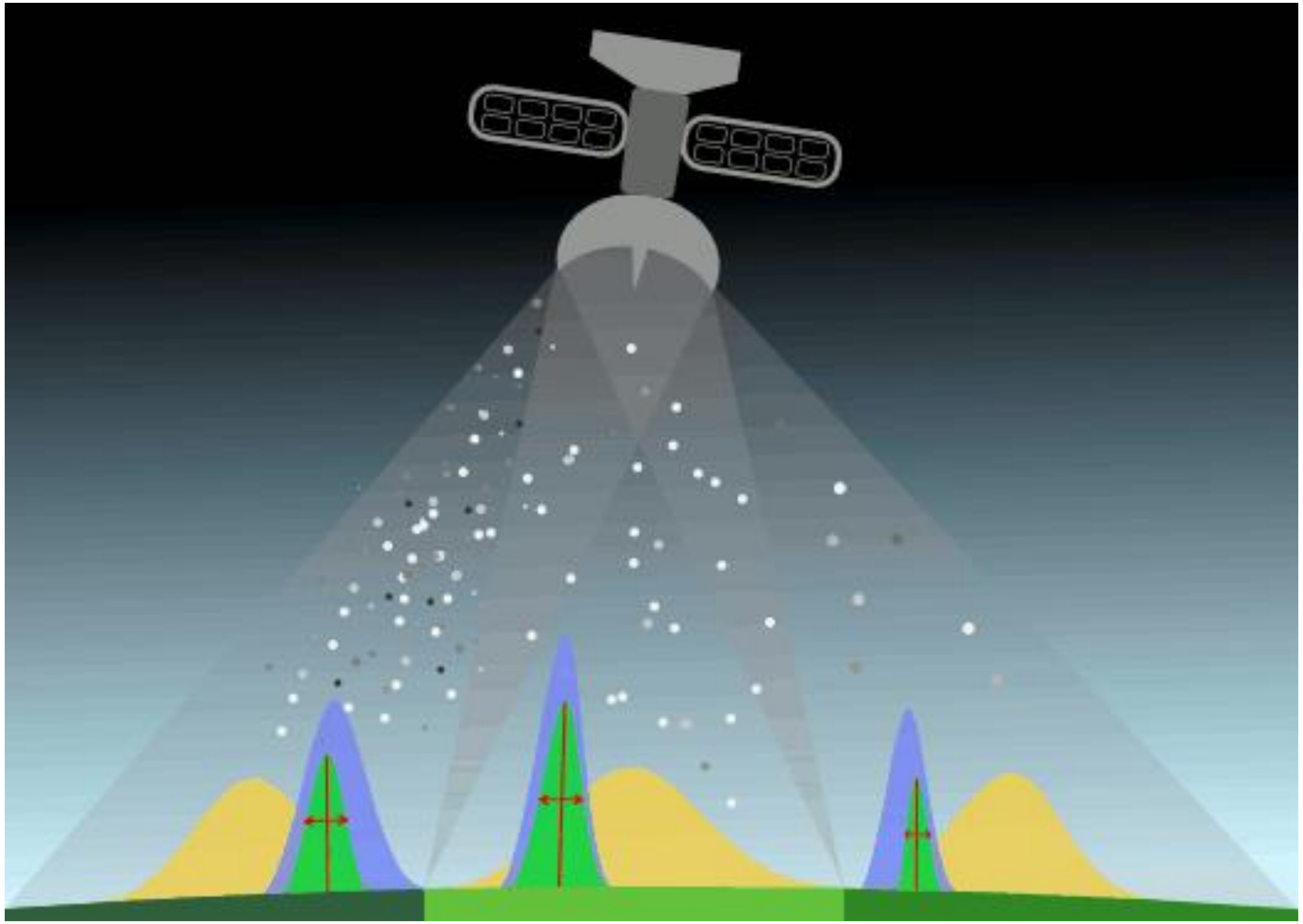
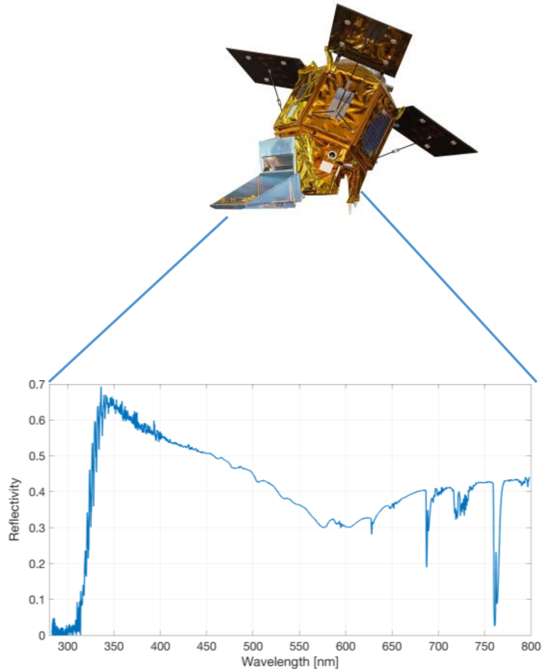
Contents of the lecture

- Basic concepts of satellite measurements at UV - VIS
- Aerosol retrievals
  - Aerosol optical depth
  - Absorbing Aerosol Index
- Trace gas retrievals
- Validation

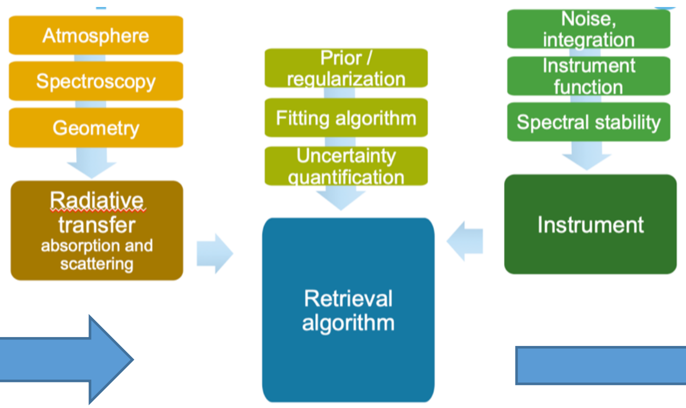


Courtesy of A. Lipponen, FMI

Basic concept of atmospheric retrievals



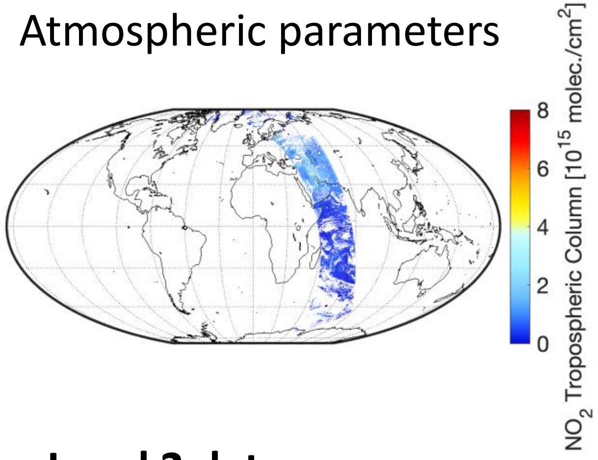
Retrieval algorithm



Level 1b data

- Products containing geolocated and calibrated spectral radiance and solar irradiance data.

Atmospheric parameters



Level 2 data

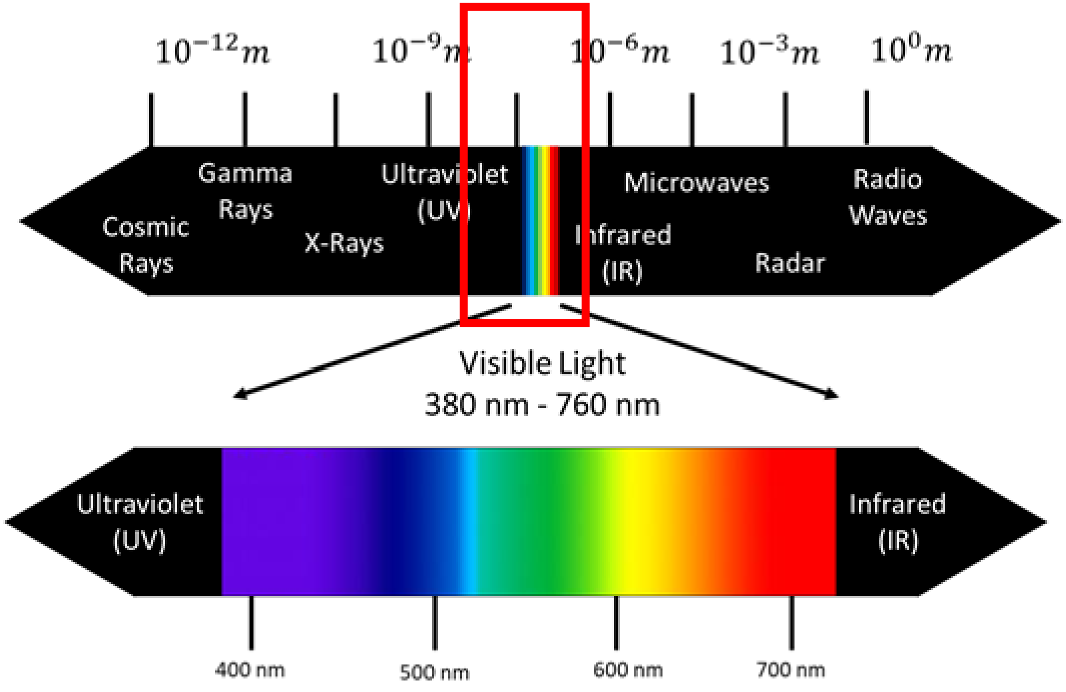
- Atmospheric products retrieved from the L1B product. Typically one file per orbit.

Level 3 data

- Globally gridded, quality flagged

Level 1 data

- UV-B, UV-A (~ 280-400 nm)
  - Some gas absorption
  - absorbing aerosols (dust, smoke, ash)
- VIS (~ 400-700 nm)
  - Aerosol information
  - Some gas absorption
  - Surface information
- IR (0.7 µm – 1 mm)
  - Many absorptions/emissions
  - Cloud information
  - water/ice separation
  - Profile information
- Microwaves(> 1 mm)
  - Moisture
  - Clouds
  - Precipitation

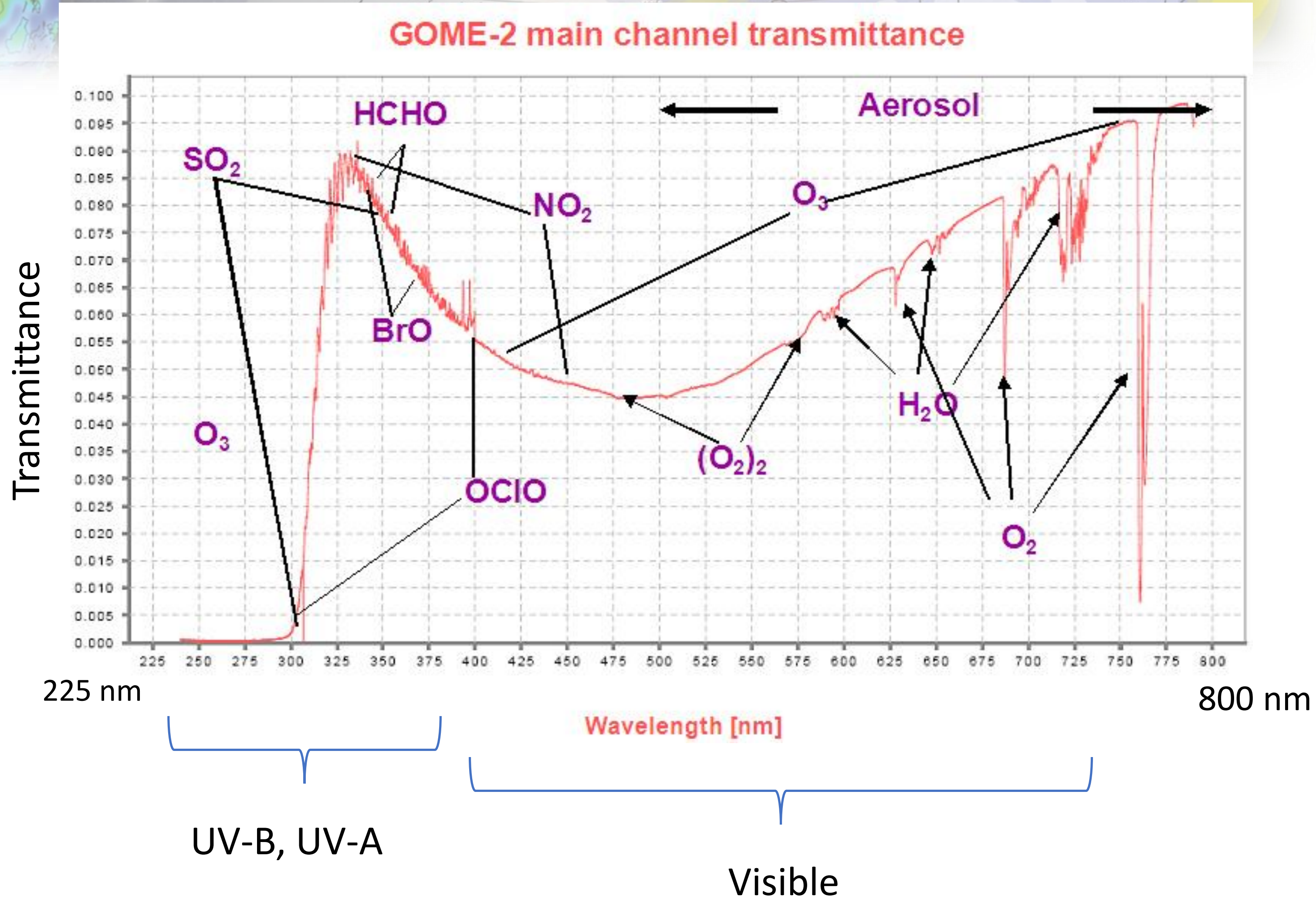


https://pressbooks.bccampus.ca/lightingforelectricians/chapter/the-em-spectrum/

Level 1 satellite observations at UV-VIS

- In theory radiation that is absorbed/scattered/emitted at any wavelengths by the atmosphere can potentially be exploited for satellite measurements of atmospheric properties

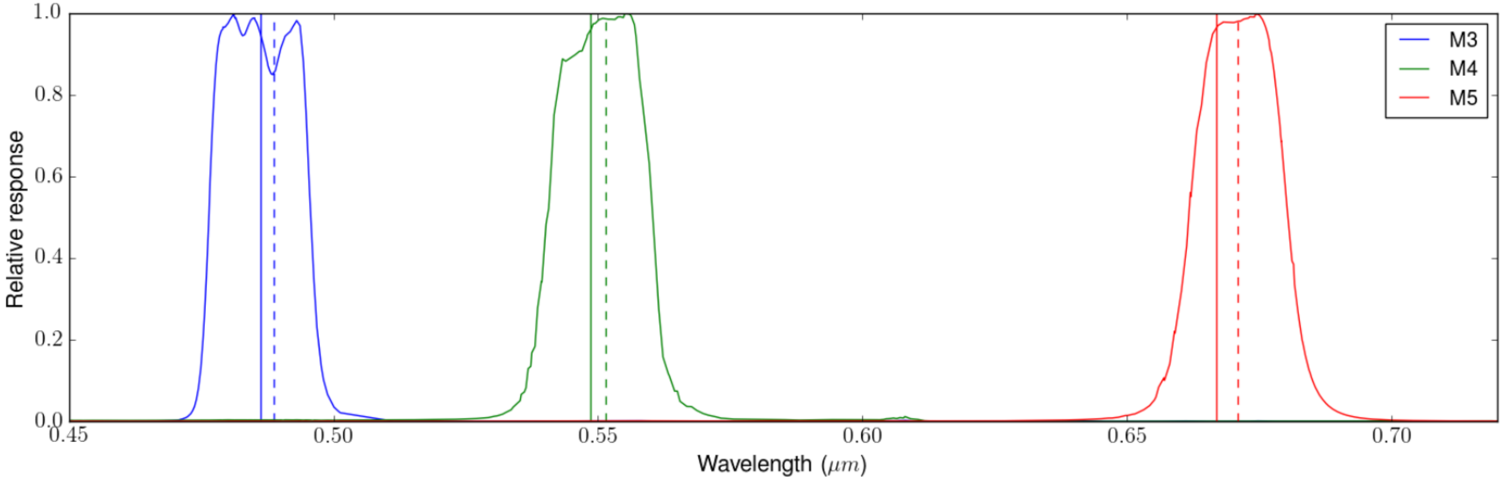
- The key is the “fingerprint” that the constituents leave to the radiation



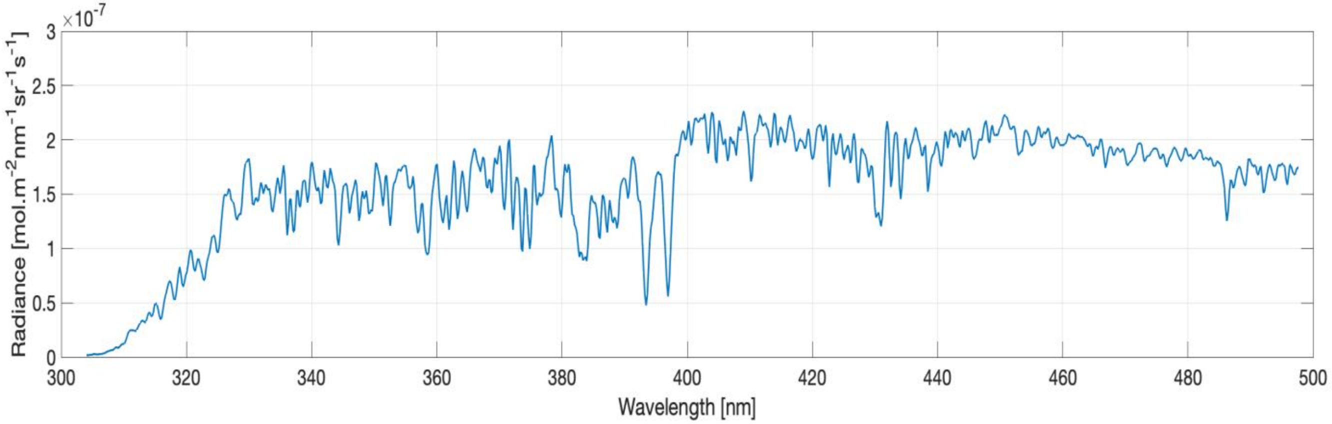
(image credit: EUMETSAT)

Level 1 Satellite measurements

Suomi NPP VIIRS
Spectral response
function

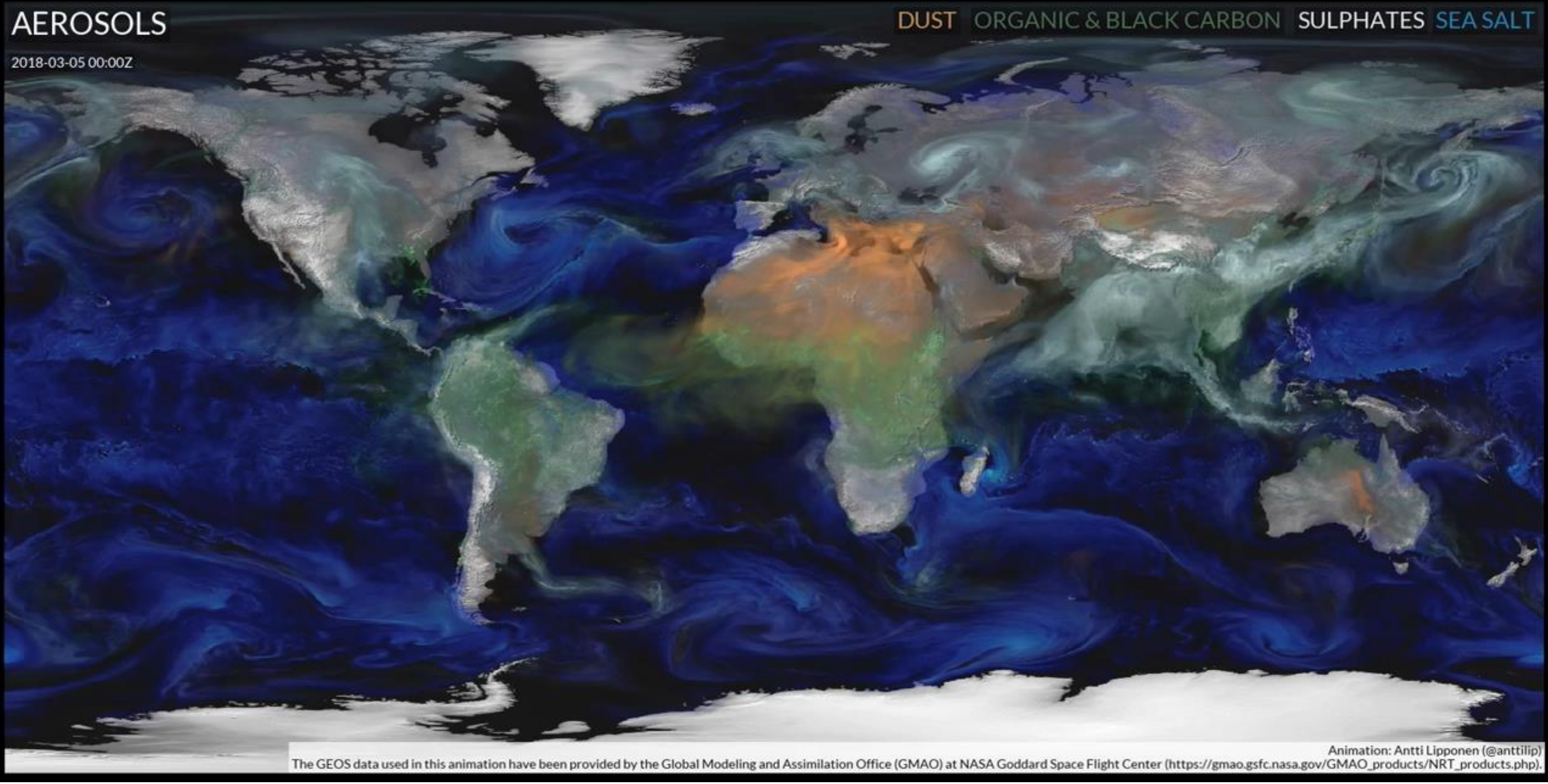


(Schreirer et al., 2018)

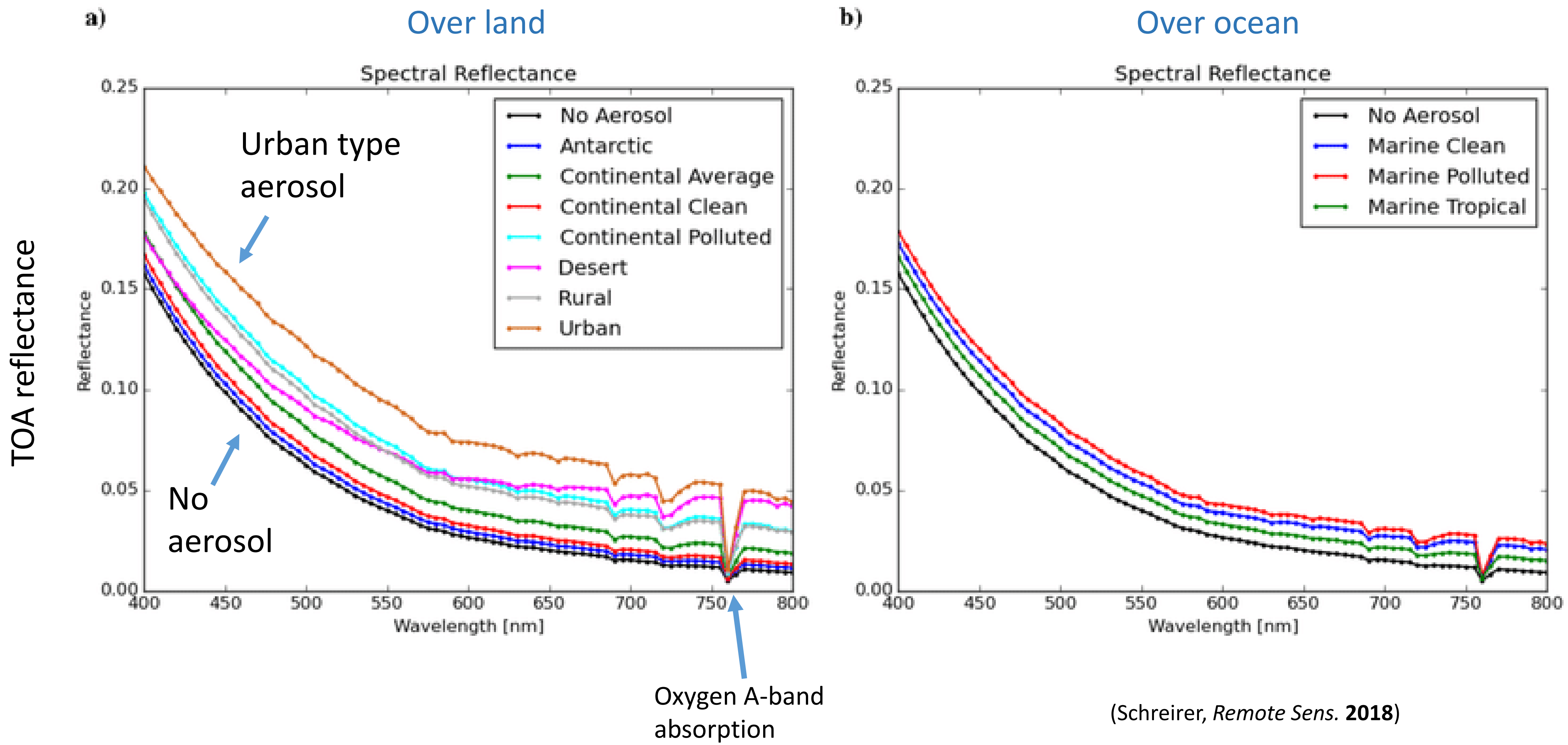


TROPOMI
L1b radiance
(one pixel)

Satellite retrieval of Aerosol Optical Depth from passive instruments


AEROSOLS
2018-03-05 00:00Z
DUST
ORGANIC & BLACK CARBON
SULPHATES
SEA SALT
Animation: Antti Lipponen (@anttilip)
The GEOS data used in this animation have been provided by the Global Modeling and Assimilation Office (GMAO) at NASA Goddard Space Flight Center (https://gmao.gsfc.nasa.gov/GMAO_products/NRT_products.php).

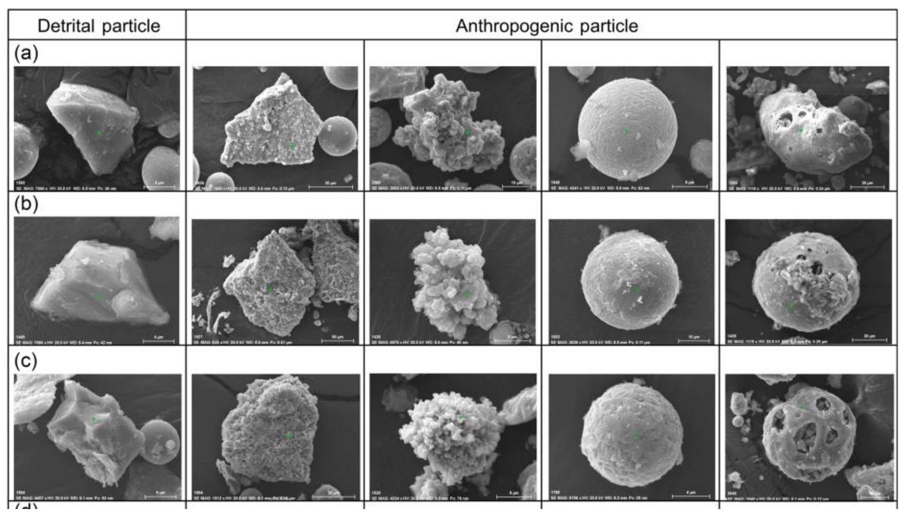
Level 1: Effect of different aerosol types on Top-of-Atmosphere (TOA) radiation at VIS



(Schreirer, *Remote Sens.* **2018**)

Aerosol optical properties

- The way how incident radiation interacts with aerosol particles depends on
  - wavelength of the radiation
  - aerosol size
  - aersol shape
  - aerosol chemical composition, defined by the complex refractive index m=n+ik



Liu et al., ACP, 2019

Scattering cross section	Absorption cross section	Single scattering albedo
C_{sca}	C_{abs}	$SSA = \frac{C_{sca}}{(C_{sca} + C_{abs})}$

Scattering cross section

C_{sca}

- Hypothetical area that is needed to collect the scattered amount of power from the incident radiation

Absorption cross section

C_{abs}

Hypothetical area that is needed to collect the absorbed amount of power from the incident radiation

Single scattering albedo

$$SSA = \frac{C_{sca}}{(C_{sca} + C_{abs})}$$

(Extinction cross section $C_{ext} = C_{sca} + C_{abs}$)

Aerosol particle size vs. wavelength

- The relationship between the size of a particle and the wavelength of the incident radiation determines which method is used to solve particle single scattering properties

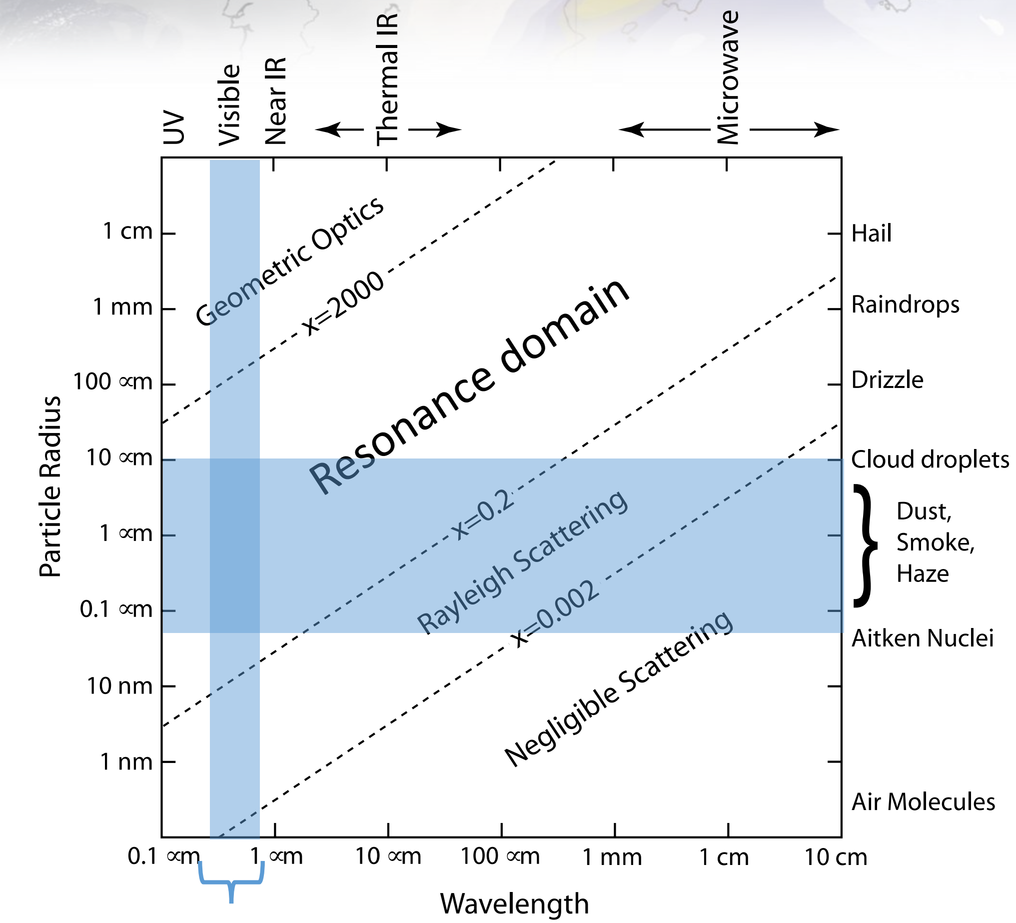
Particle diameter

Size parameter

$$x = \frac{D_p \pi}{\lambda}$$

wavelength

- VIS wavelengths are good for AOD retrievals because the atmosphere is nearly transparent
  - Resonance domain: solving particles’ single scattering properties is complex
  - Methods: Mie, T-matrix, DDA



Suitable wavelength range for satellite observations

(modified from G.Petty, 2006)

Aerosol optical depth (AOD)

- Also known as aerosol optical thickness (AOT), most commonly retrieved aerosol parameter from satellites
- AOD is related to the amount of (optically active) aerosols in a total atmospheric column.
- Extinction coefficient:

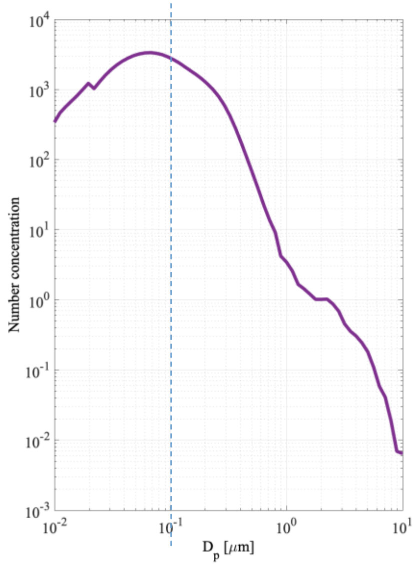
$$b_e = b_a + b_s$$ units of inverse length [m^{-1}]

AOD is defined as the sum of aerosol extinction at all atmospheric levels, from surface up to the top of the atmosphere

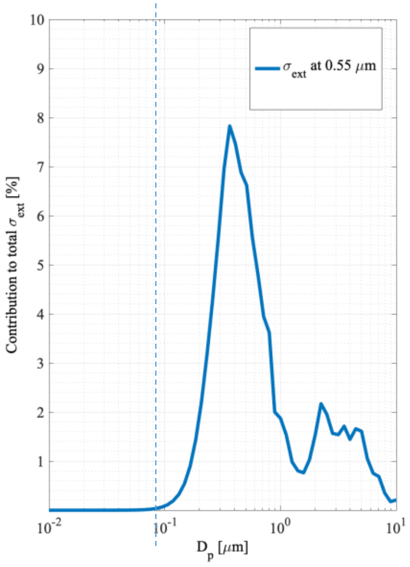
$$AOD = \int_{surf}^{TOA} b_e(s)\,ds$$

[unitless]

Measured aerosol size distribution



Contribution of each particle size to the total extinction at 550 nm



AOD retrievals

$$\rho_\lambda^{\mathrm{TOA}}(\tau,\theta_0,\theta,\varphi) = \rho_\lambda^{a}(\tau,\theta_0,\theta,\varphi) + \frac{T_\lambda(\tau,\theta_0)\,T_\lambda(\tau,\theta)\rho_\lambda^{s}}{1 - s_\lambda(\tau)\rho_\lambda^{s}}$$

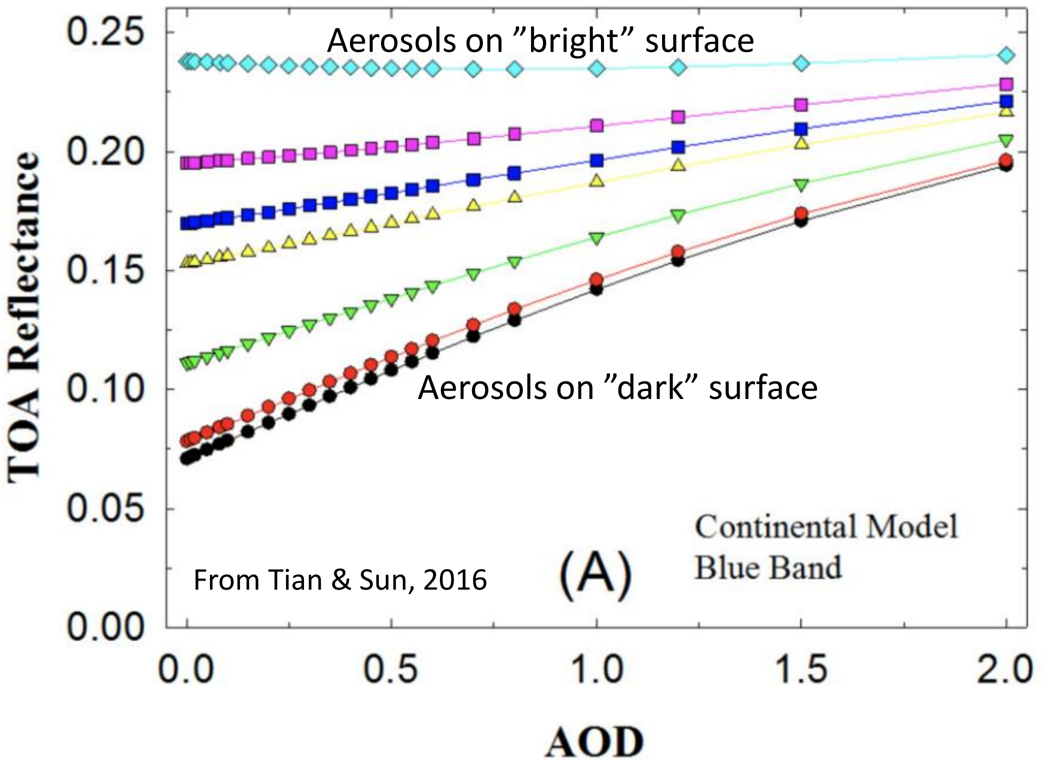
Reflectance at TOA measured by satellite

Atmospheric path reflectance:
- aerosols
- molecules

Surface contribution

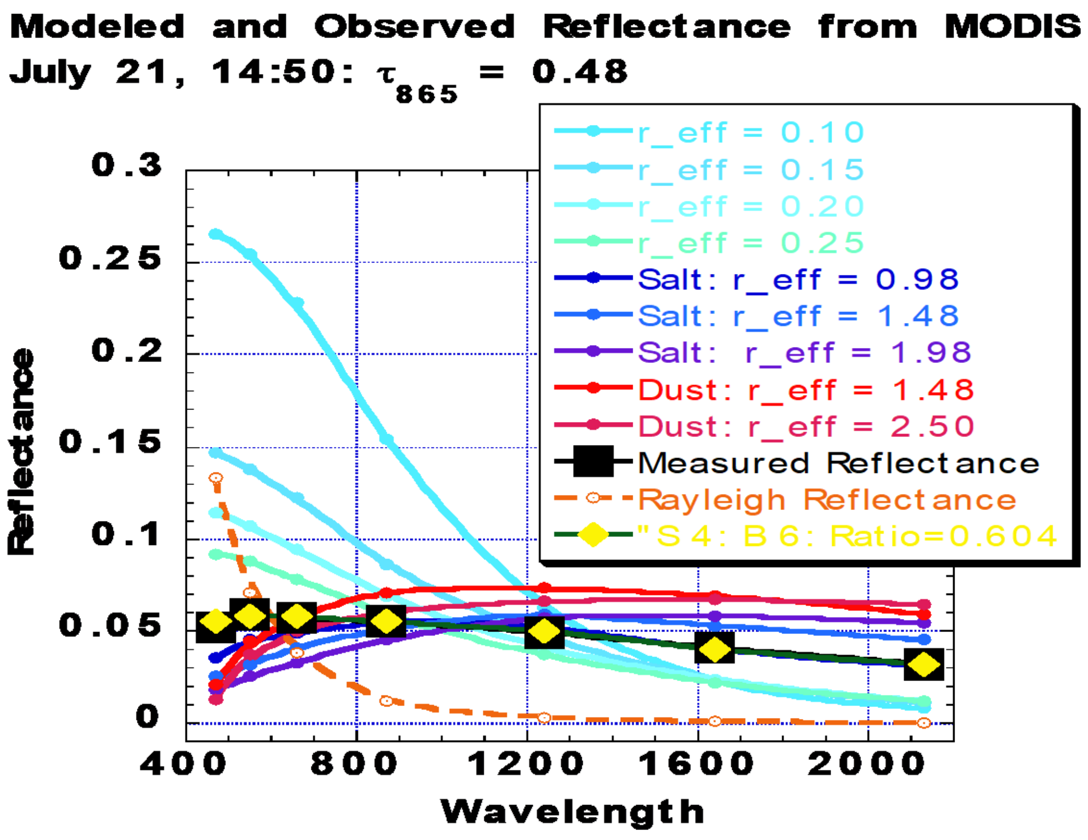
- Aim: to separate the aerosol contribution from the measured TOA reflectance:
  - **Cloudscreening -> very important step in the retrieval**
  - Surface contribution (can be also retrieved simultaneously with aerosols)
  - Rayleigh correction

Aerosols + surface



Pre-computed Look-Up-Tables

- Full radiative transfer calculation for pixel by pixel would be computationally impossible.
- AOD retrievals often utilizes so called look-up-tables (LUTs) in the retrieval
- Basic LUT's: consider different aerosol scenarios and model $\rho_{\lambda,aer}^{TOA}$ as a function of satellite-sun viewing geometry and wavelength.
- Aerosol retrievals can utilize several LUTs, where each LUT represents a certain aerosol "type" (i.e. size distribution & composition)



(Levy, 2007)

Example of an AOD retrieval scheme

Modeled TOA reflectance

TOA reflectances are simulated by mixing the reflectances corresponding to two different aerosol models:

$$\rho_\lambda^{\mathrm{TOA}} = \eta \rho_\lambda^{TOA,f} + (1-\eta)\rho_\lambda^{TOA,c}$$

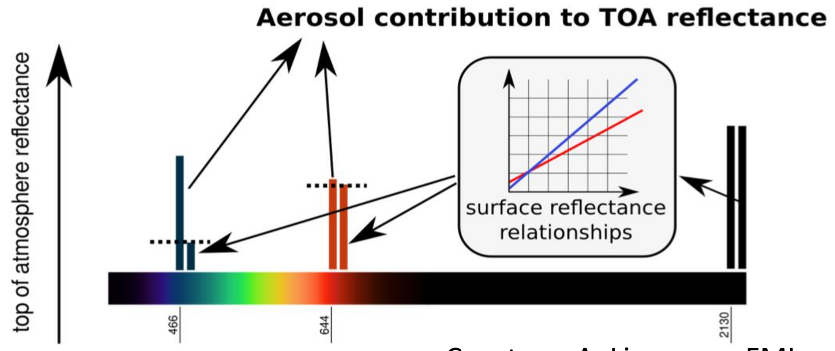
Fine mode fraction

Pre-computed Look-Up-Tables for different fine/coarse mode aerosol

- Climatologies can be used to select models by location / season

Measured TOA reflectance

Cloud screening

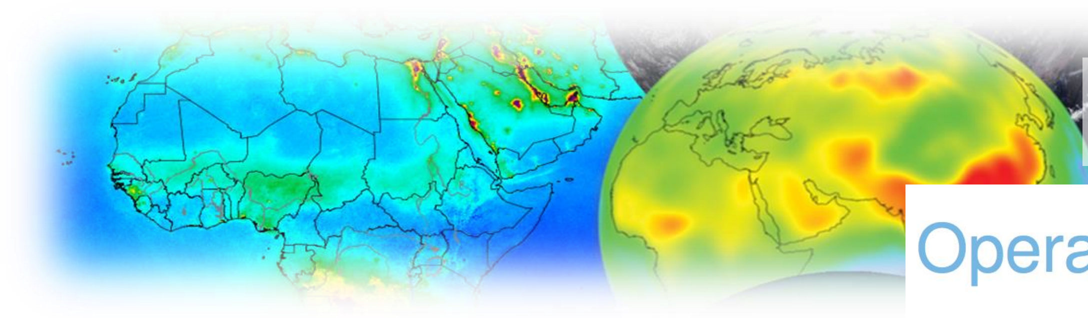


Courtesy: A. Lipponen, FMI

466 nm 644 nm 2130 nm

- linear surface reflectance relationships obtained at 2.1 µm are used to get an estimate for the surface reflectances at shorter wavelengths

Select the combination of AOD and FMF that minimizes the difference between measured and modeled spectral ρ^{TOA}

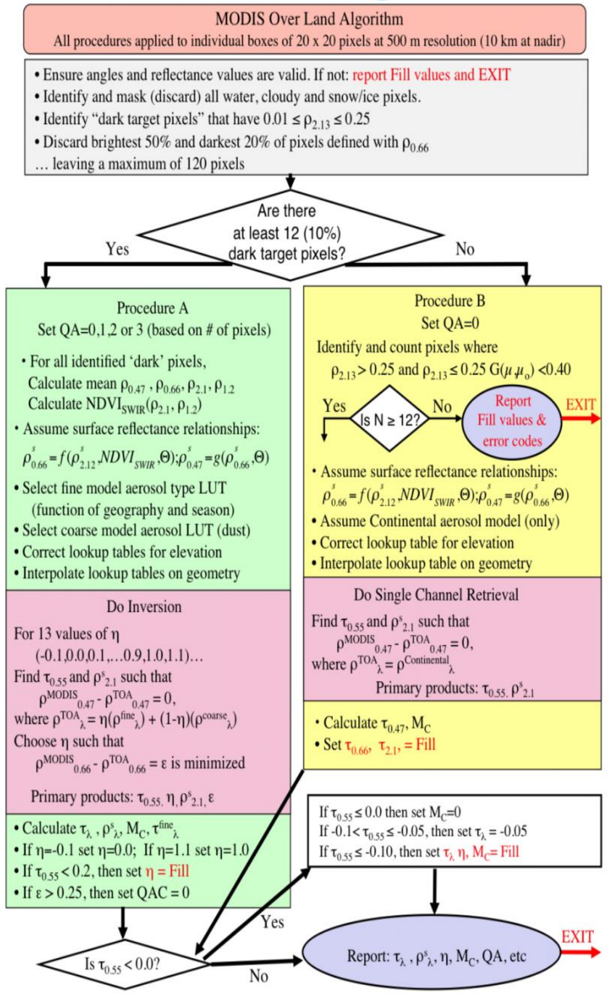


Examples of AOD retrieval algorithms

AOD is available from several instruments and algorithms:

- MODIS Terra & Aqua; Dark Target, Deep Blue
- VIIRS (Suomi NPP, NOAA-20)
- MISR
- SeaWiFS
- AVHRR
- AATSR
- SLSTR (Sentinel-3)
- PMap (Merged from multiple instruments)
- …

Operational Dark Target



Bayesian Aerosol Retrieval (BAR)

Algorithm is based on operational MODIS Dark Target over Land algorithm

All pixels in a granule are retrieved simultaneously

Statistical (Bayesian) framework for inverse problems

No surface reflectance relationship needed

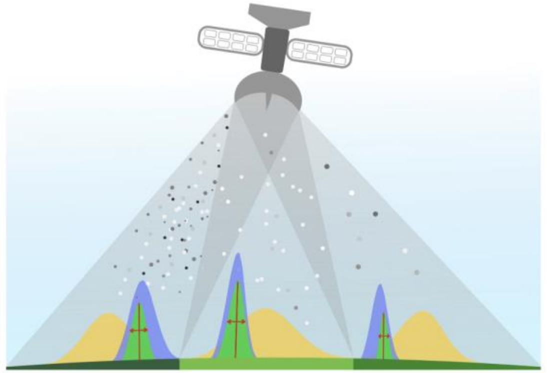
Quantities retrieved
- AOD
- FMF
- Surface reflectances

Approximation error model

Prior distribution
- Spatial correlations
- Seasonality
- Multivariate normal distributions
- Non-negative AOD

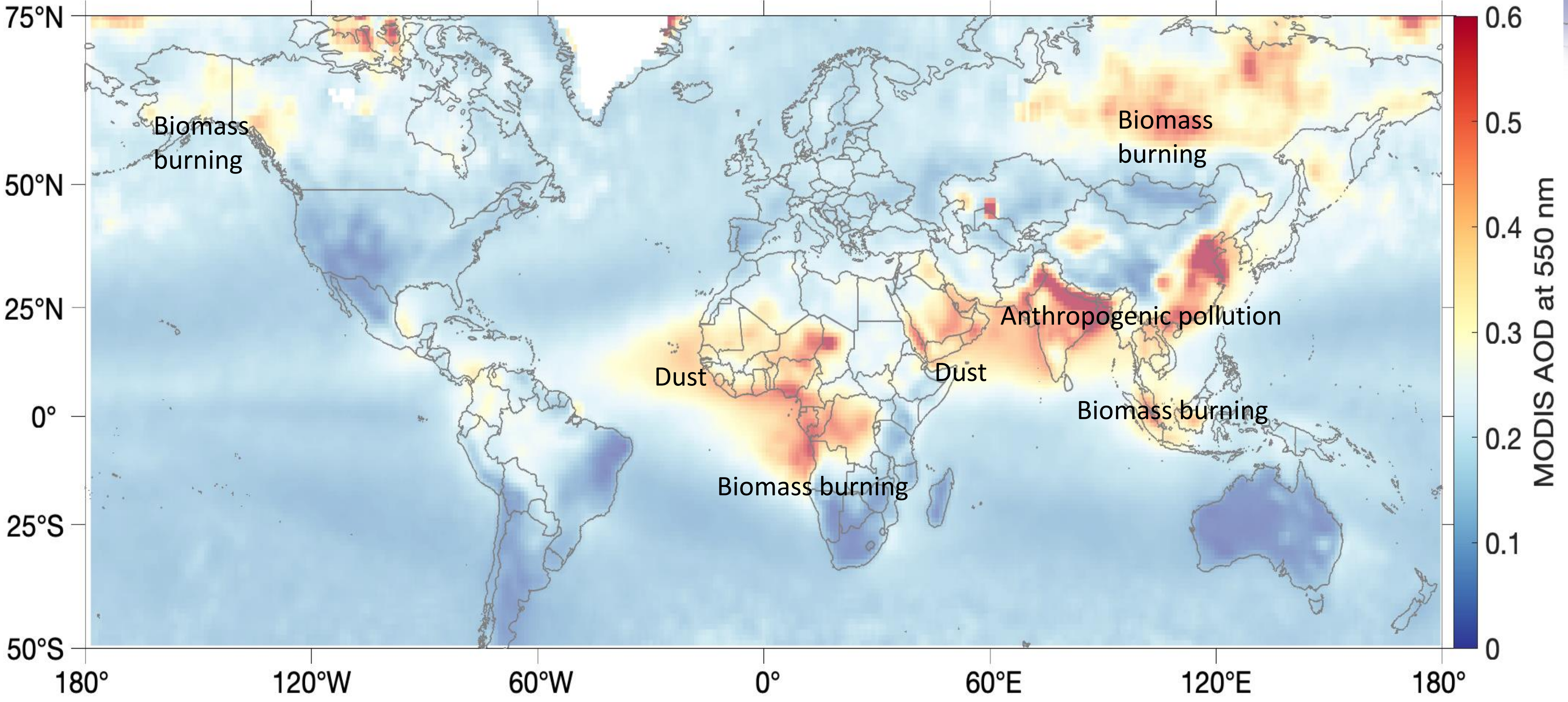
Likelihood distribution
- Connects observations to unknowns
- Observation model (Dark Target LUT)
- Uncertainty models

Posterior distribution
- Solution to our retrieval
- Most probable values as retrievals
- Pixel level uncertainty



Lipponen et al., AMT, 11, 1529–1547, 2018

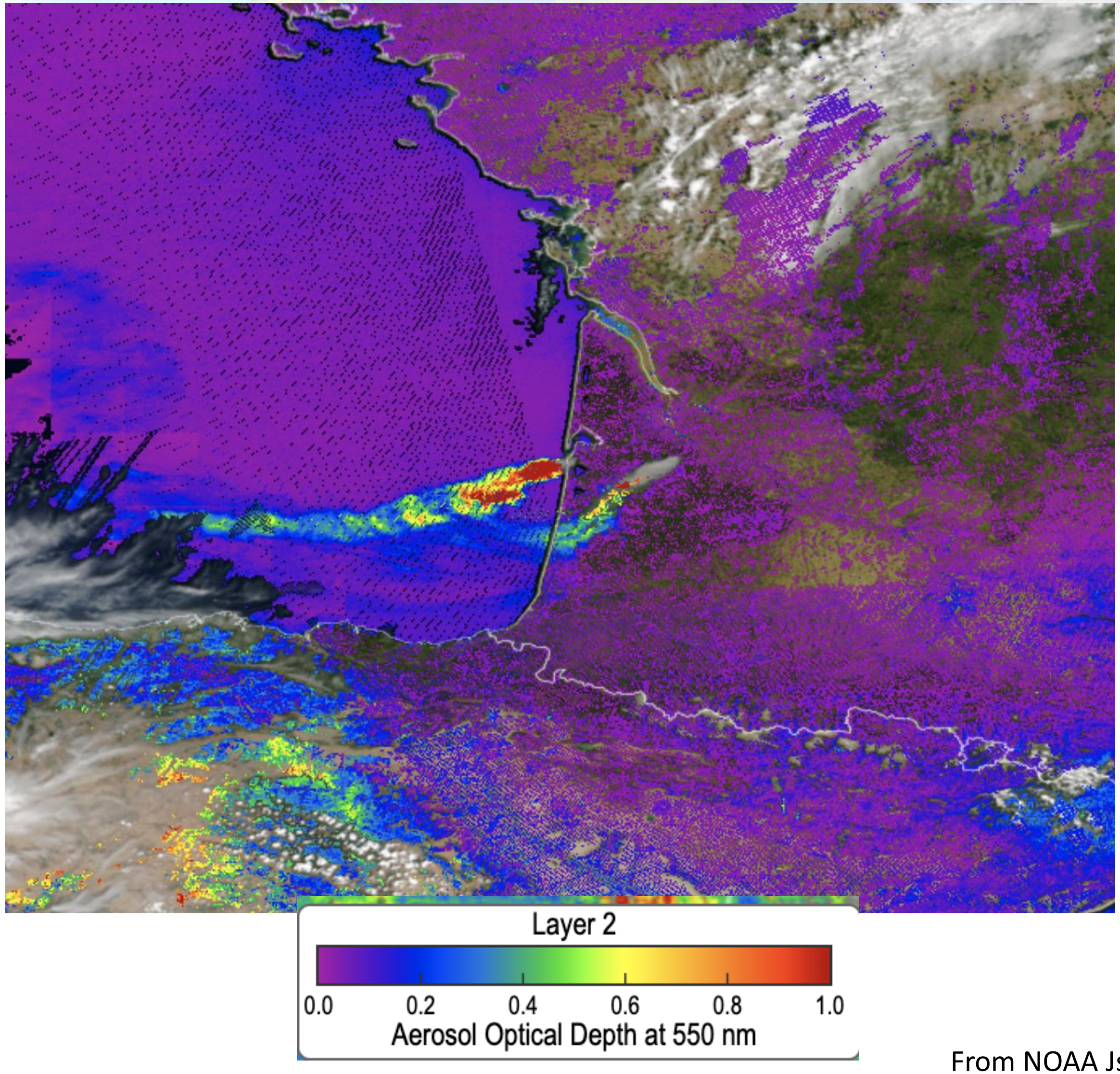
MODIS Terra AOD (at 550 nm) 2019



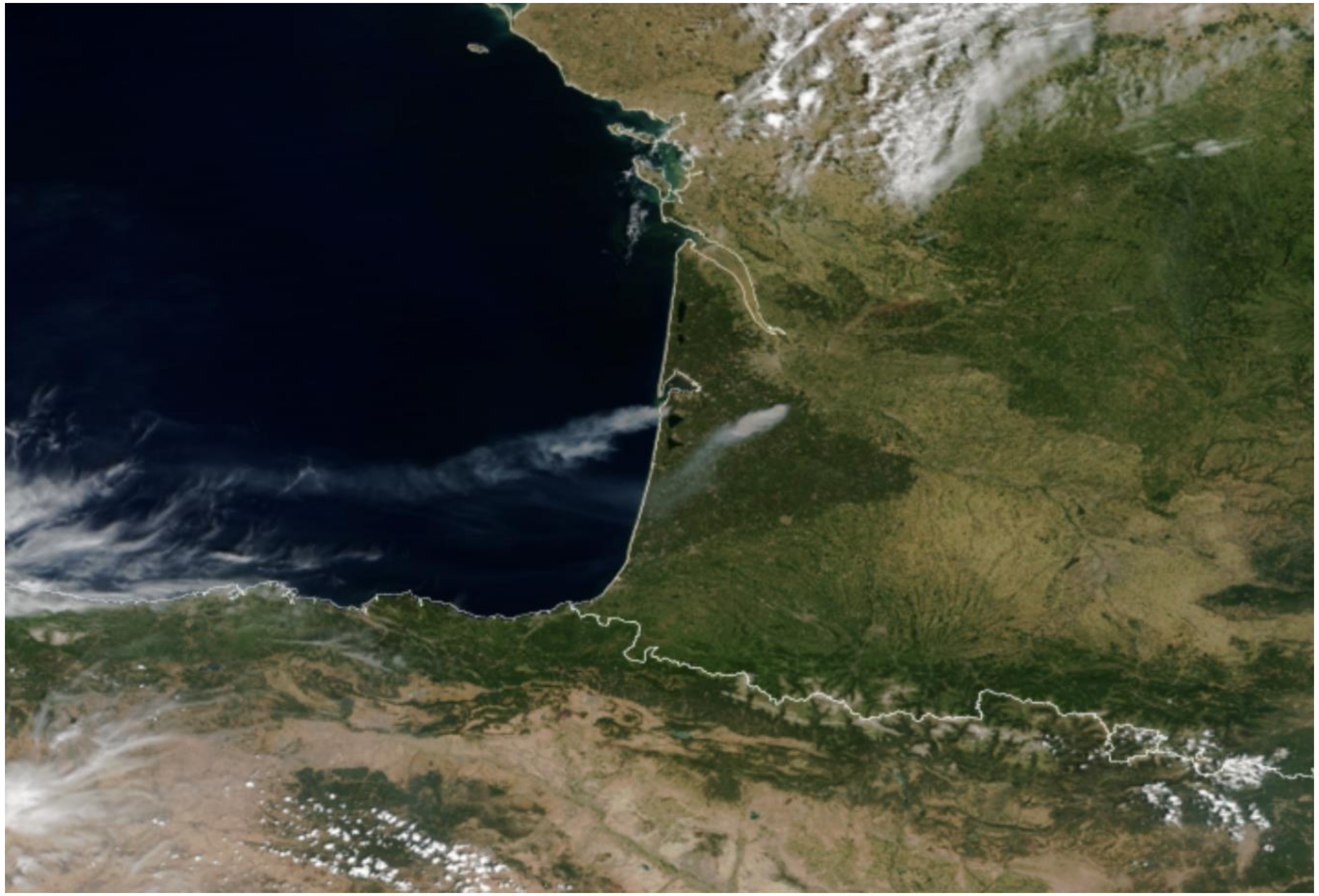
- Global mean AOD at 550 nm: about 0.15
- Typical range of variation at 550 nm: 0.05…2.0
- AOD timeseries of > 20 years are available (e.g. Sogacheva et al. 2020)

Example: Wildfires in Southern France 13.7.2022

Suomi NPP/VIIRS AOD at 550 nm



Suomi NPP/VIIRS RGB

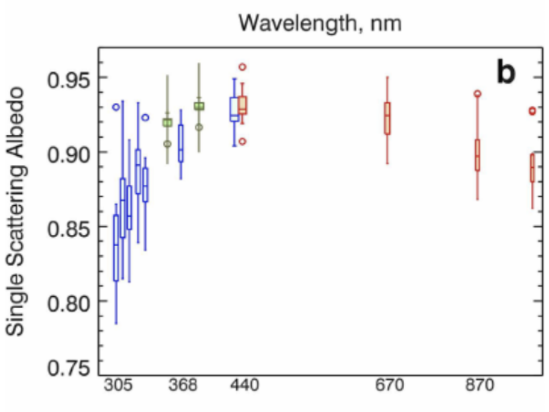


From NOAA Jstar Mapper

Absorbing Aerosol Index

- AAI, also referred as UVAI or AI is an **index** that indicates the presence of absorbing aerosols (dust, smoke, volcanic ash)
- AAI is not a “classical satellite retrieval” because spectrum is not fitted.
- In the UV/VIS wavelength range, the AAI is not sensitive to surface type and is defined in the presence of clouds
- The AAI has few requirements as doesn’t depend on a priori information and only few external parameters are needed for calculation.

Smoke single scattering albedo



Mok et al, sci. rep. 6, 2016

AAI residue method

$$r_\lambda = -100 \cdot \left\{ {}^{10}\log\left(\frac{R_\lambda}{R_{\lambda 0}}\right)^{meas} - {}^{10}\log\left(\frac{R_\lambda}{R_{\lambda 0}}\right)^{Ray} \right\}$$

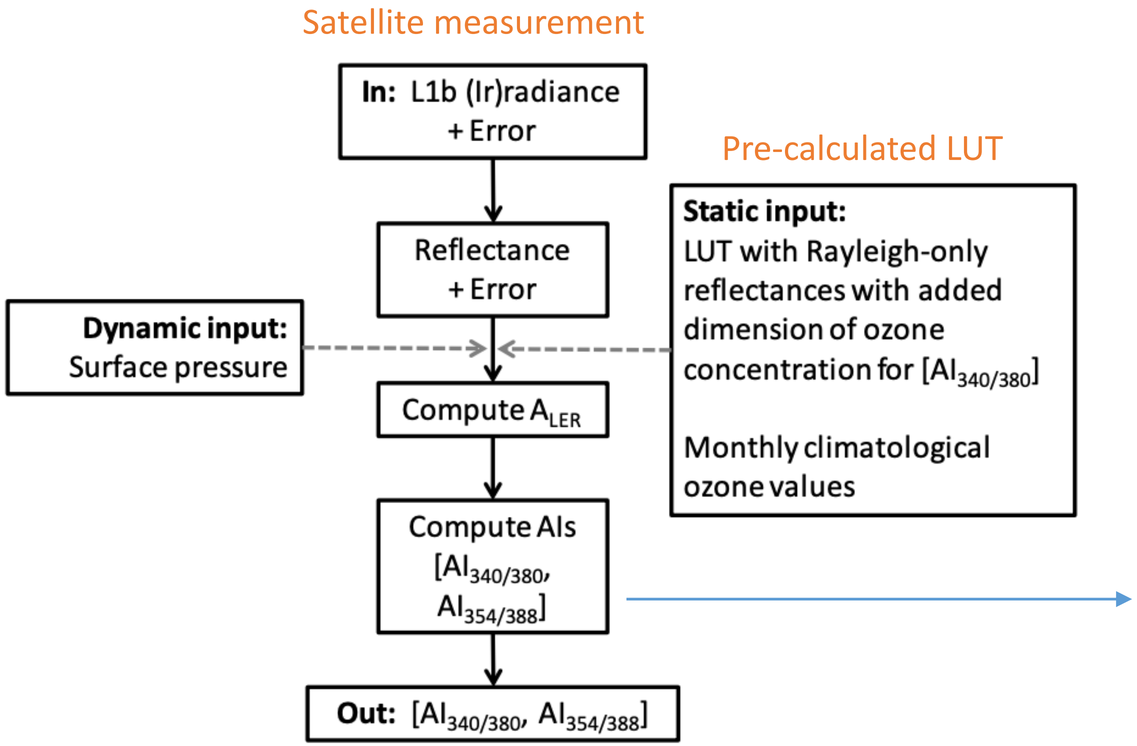
Radiance at TOA measured by the satellite at wavelength λ

- Real atmosphere including aerosol contribution

Modeled TOA radiance for aerosol-free atmosphere

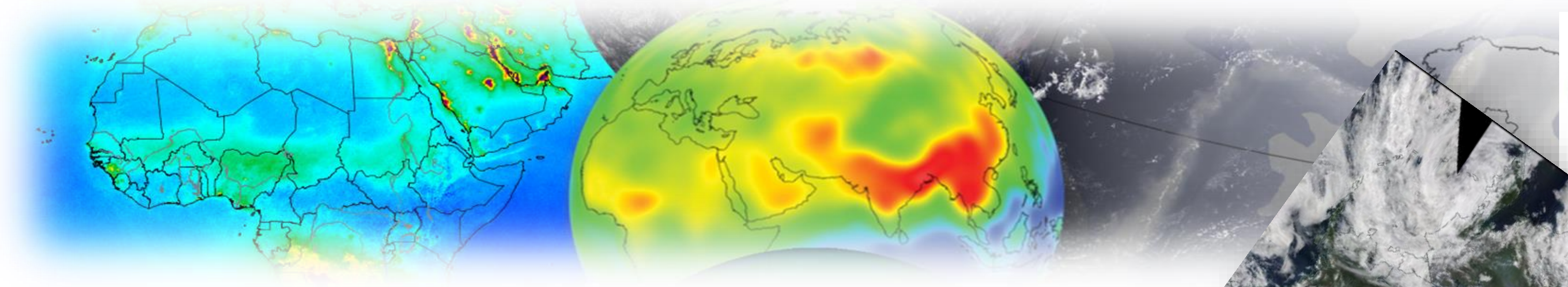
- Incl. Rayleigh scattering and absorption, and
- surface reflection and absorption.

Example of TROPOMI AAI retrieval scheme:



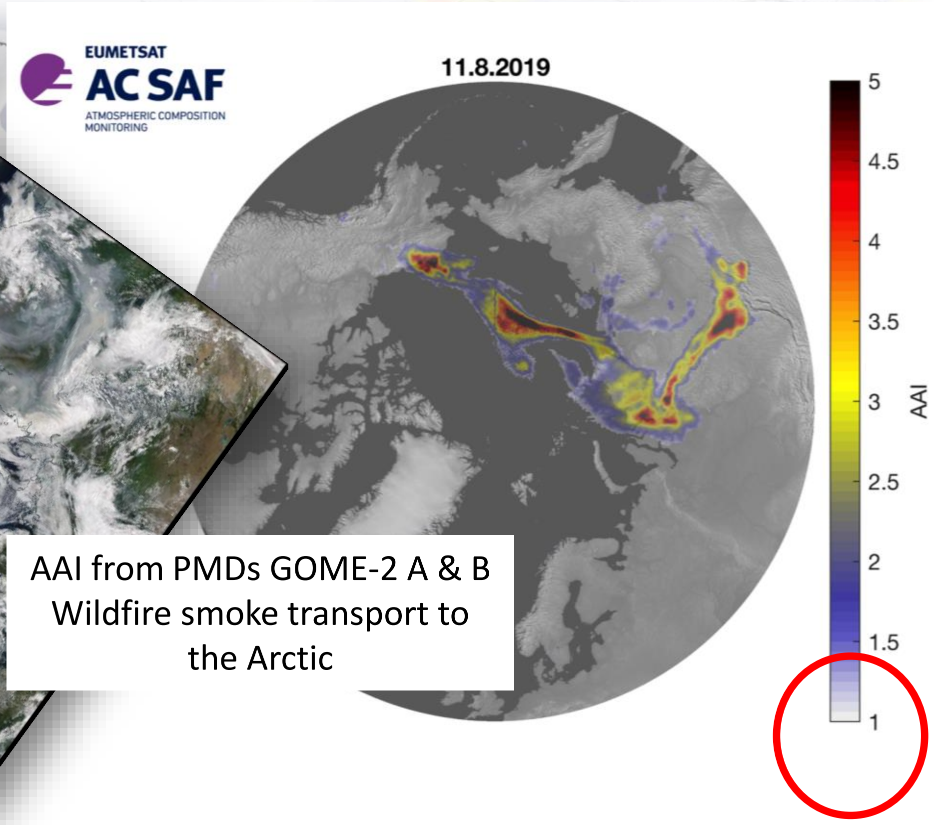
- AAI is defined from reflectance pairs measured at two different wavelengths.
- The key assumption in the AAI computation is that surface albedo (A_{LER}) is assumed constant between the two wavelenghts λ_1 and λ_2

$$AI = 100 \cdot \log_{10}\left(\frac{R_{calc}(\lambda_1, A_{LER}(\lambda_2))}{R_{meas}(\lambda_1)}\right)$$



- Positive values of AAI (>0.5) indicate presence of absorbing aerosols
  - Sensitivity mostly to elevated layers
- AAI is a function of many parameters, and cannot be used as direct measure of aerosol amount.
  - AAI depends e.g. on aerosol type (SSA), aerosol amount (AOD), height of the aerosol layer.

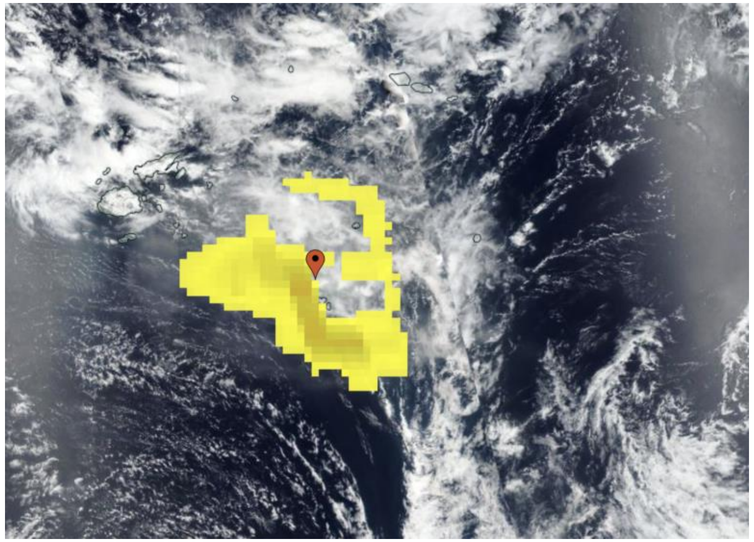
- Highly positive AAI values should be foremost considered as an indication of the presence of absorbing aerosols
  - AAI values are not necessarily comparable from case to case



AAI from PMDs GOME-2 A & B
Wildfire smoke transport to the Arctic

Volcanic ash from Hunga Tonga eruption
SNPP / OMPS

15.1.2022



Trace gas retrievals

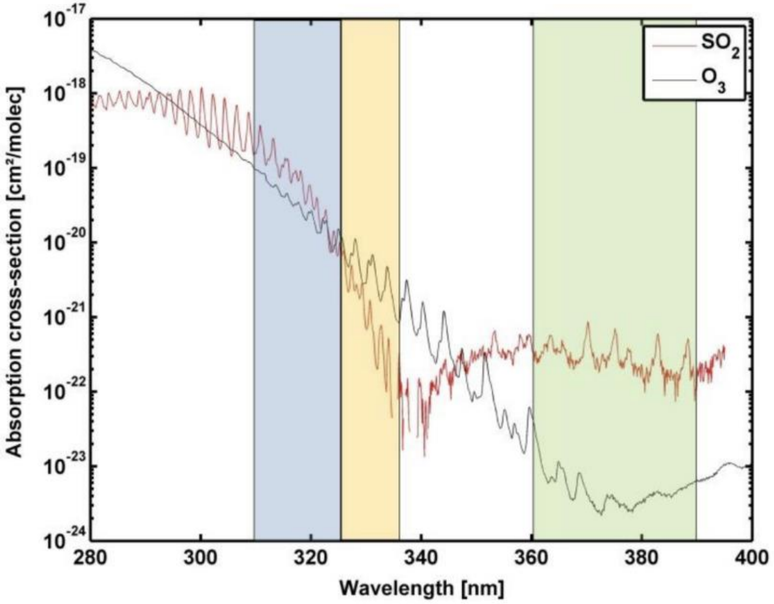
Gas absorption

Absorption cross section $\sigma = \dfrac{total\ absorbed\ energy/unit\ time}{total\ incident\ intensity\ (energy/unit\ time/area)}$ [cm^2 /molec.]

Physical interpretation: Effective area of the molecule that photon needs to traverse in order to be absorbed.

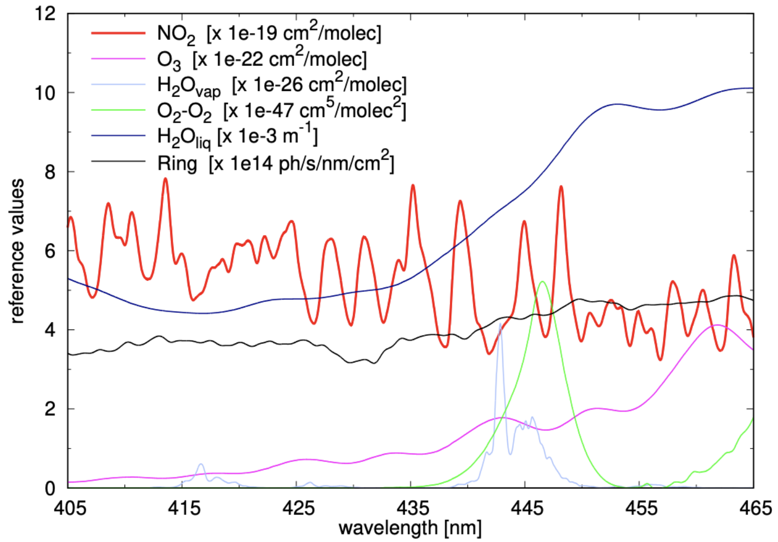
SO_2 and O_3 absorption cross sections

(coloured boxes SO_2 fitting windows for TROPOMI)



Tropomi SO_2 ATBD

Gas absorption cross sections (scaled) in the NO_2 fitting window



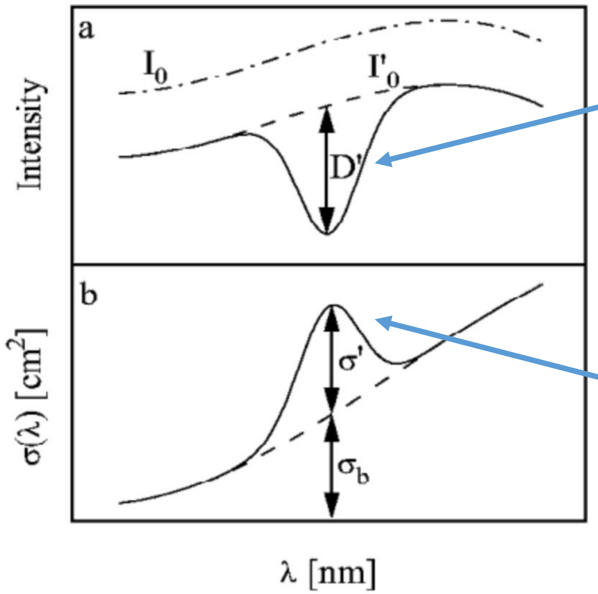
TROPOMI NO2 ATBD

Differential Optical Absorption Spectroscopy (DOAS)

- DOAS is the most widely used method to derive atmospheric trace gas constituents in the UV–VIS, based on absorption spectroscopy
- The key idea of the DOAS principle is to separate high and low frequency components of the reflectance spectrum
  - Can resolve multiple gases simultaneously
  - Differential cross section => high frequency component
- Basis: Lambert Beer's law:

$$I = I_0 * \exp(-\sigma * c * L)$$

  - σ: cross section
  - c: concentration of absorber
  - L: light path through absorber



Reduction in intensity

Due to differential absorption cross section of an atmospheric trace gas

Credit: volkamergroup.colorado.edu/research/experimental-tools/doas

The DOAS equation

Integral over light path ds

$$I(\lambda,\Theta) = \alpha(\lambda,\Theta) I_0(\lambda) exp\left\{ -\int \left(\sum_{j=1}^{J} \sigma_j(\lambda)\rho_j(s) + \sigma_{Msca}(\lambda)\rho_{Msca}(s) + \sigma_{Rsca}(\lambda)\rho_{Rsca}(s) \right) ds \right\}$$

Intensity measured by the instrument

Scattering efficiency

Unattenuated intensity

Attenuation:

- absorption by trace gas j
- Mie scattering
- Rayleigh scattering

Slant column

$$SC_j = \int \rho_{j(\lambda)} ds$$

Integrated total amount of absorber j along the light path s

- Scattering terms vary smoothly with wavelenght
- Also absorption cross sections can be separated into low and high frequency parts

$$\sigma = \sigma_{low} + \sigma'$$

Approximate low fequency varying parts with low order polynomials

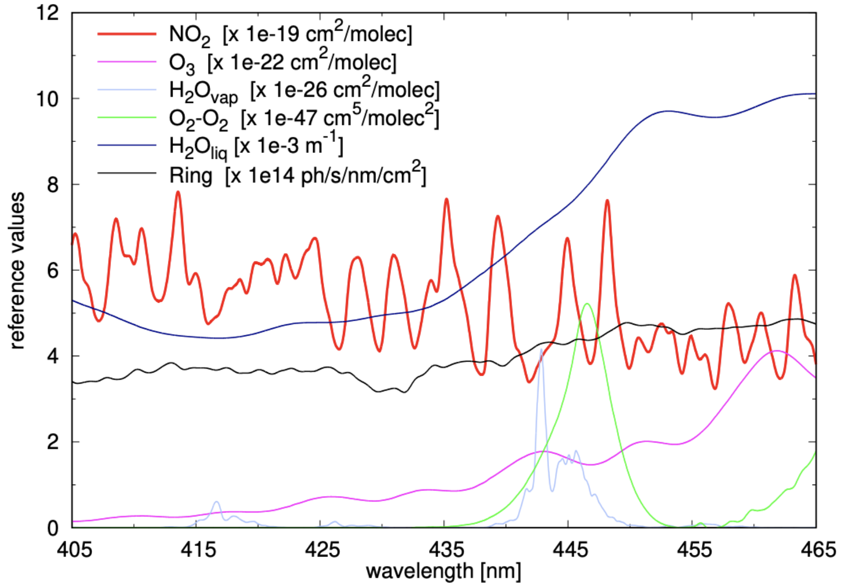
$$\ln\left(\frac{I(\lambda,\Theta)}{I_0(\lambda,\Theta)}\right) = -\sum_{j=1}^{J} \sigma *_j (\lambda)\, SC_j + \sum_{p} b_p \lambda^p$$

Polynomial

Sum of all tracers that influence in the measurement window

Fitted

- For different trace gas retrievals the DOAS equation can be somewhat modified
  - E.g. correction for the Ring effect, non-linear effects in the retrieval
- DOAS (least squares) fitting between measured and modeled reference spectra
- Result: slant column of the trace gas of interest + number of auxiliary parameters and error diagnostics



Example of NO_2 spectral measurement window

TROPOMI ATBD

Air Mass Factor

- Air mass factor M is the ratio of the retrieved slant column S to the vertical column V in the atmosphere

$$M = \frac{S}{V}$$

- AMF is defined with a radiative transfer code, and it depends on:
  - Viewing geometry and wavelength
  - Vertical distribution of the absorber
  - Clouds
  - Aerosols
  - Surface albedo

Altitude dependent AMF for individual layer l

$$M = \frac{\sum_l m_l(\mathbf{b}) x_l c_l}{\sum_l x_l}$$

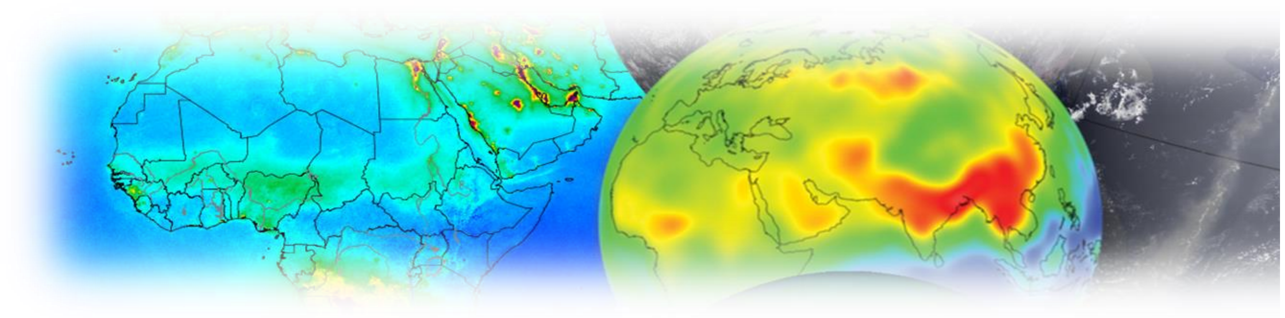
Layer spec. corr. factor, e..g.for T

Partial gas column in layer l

DOAS-type averaging kernel:

- Information on measurement vertical sensitivity

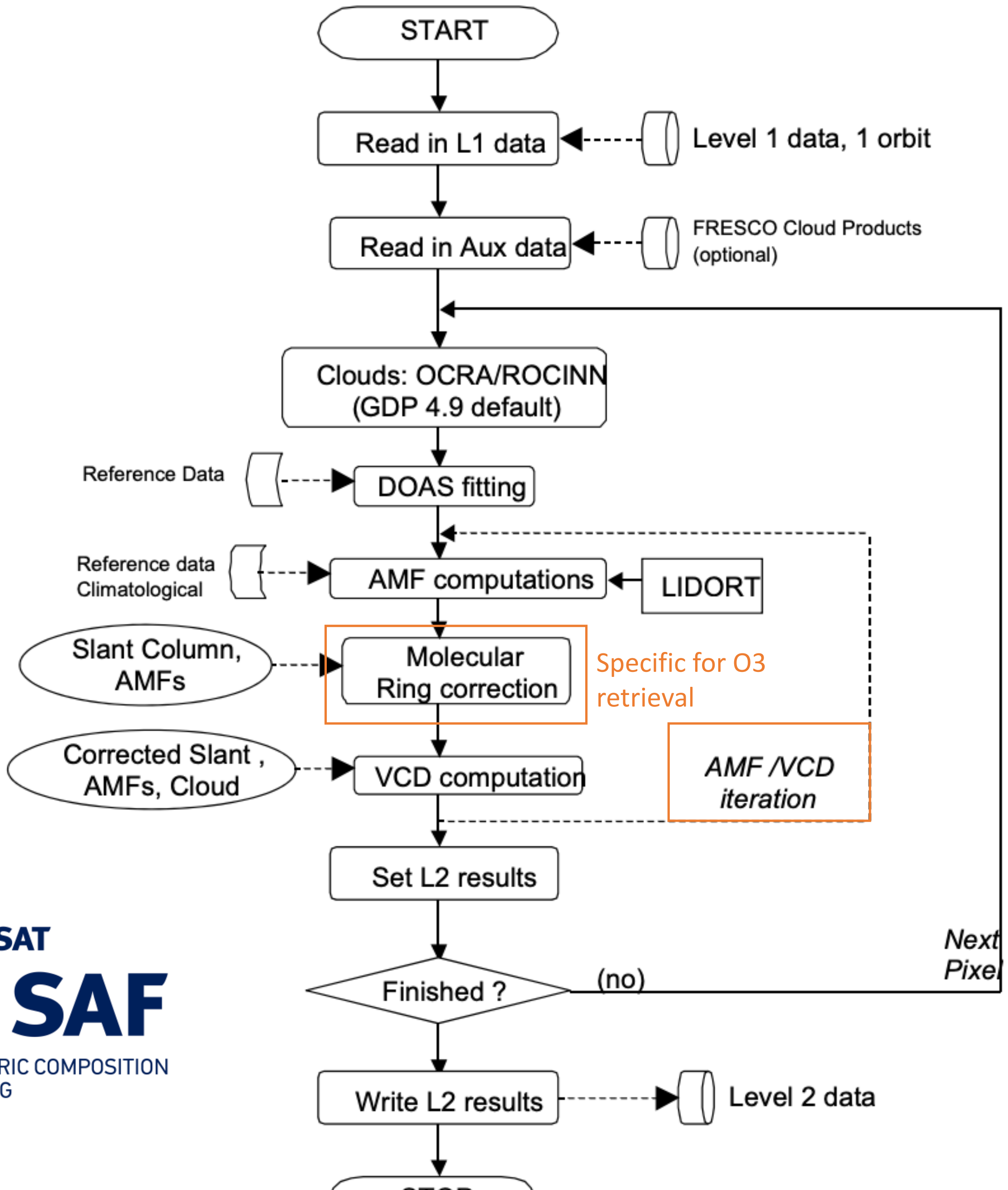
$$A_l = \frac{m_l}{M_t}$$



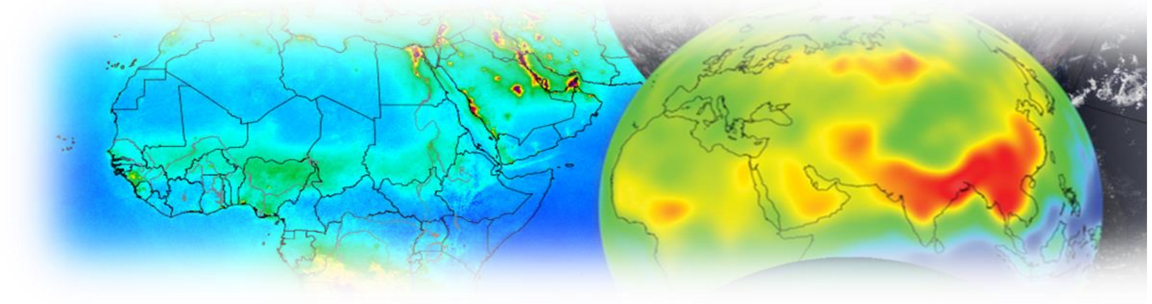
Example: The GDP algorithm for operational GOME-2 trace gas retrievals

Product	Wavelength region
Ozone column	325.0-335.0 nm
NO_2 column*	425.0-450.0 nm
BrO column	332.0-359.0 nm
HCHO column	328.5-346.0 nm
SO_2 column**	312.0-325.0 nm
H_2O column	614.0-683.2 nm
OClO column***	345.0-389.0 nm

EUMETSAT AC SAF ATMOSPHERIC COMPOSITION MONITORING

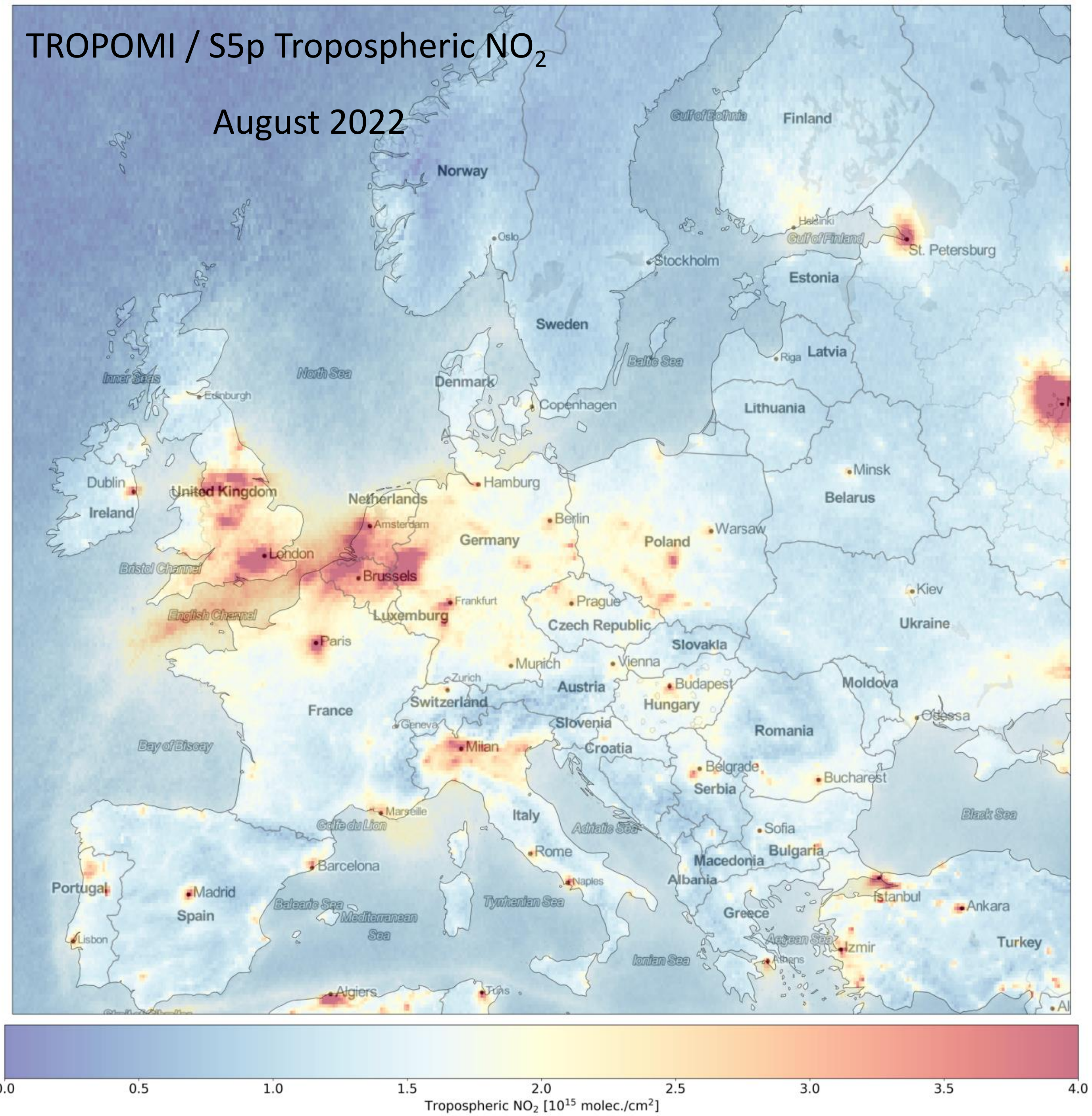


Van Roozendael et al. (2006)



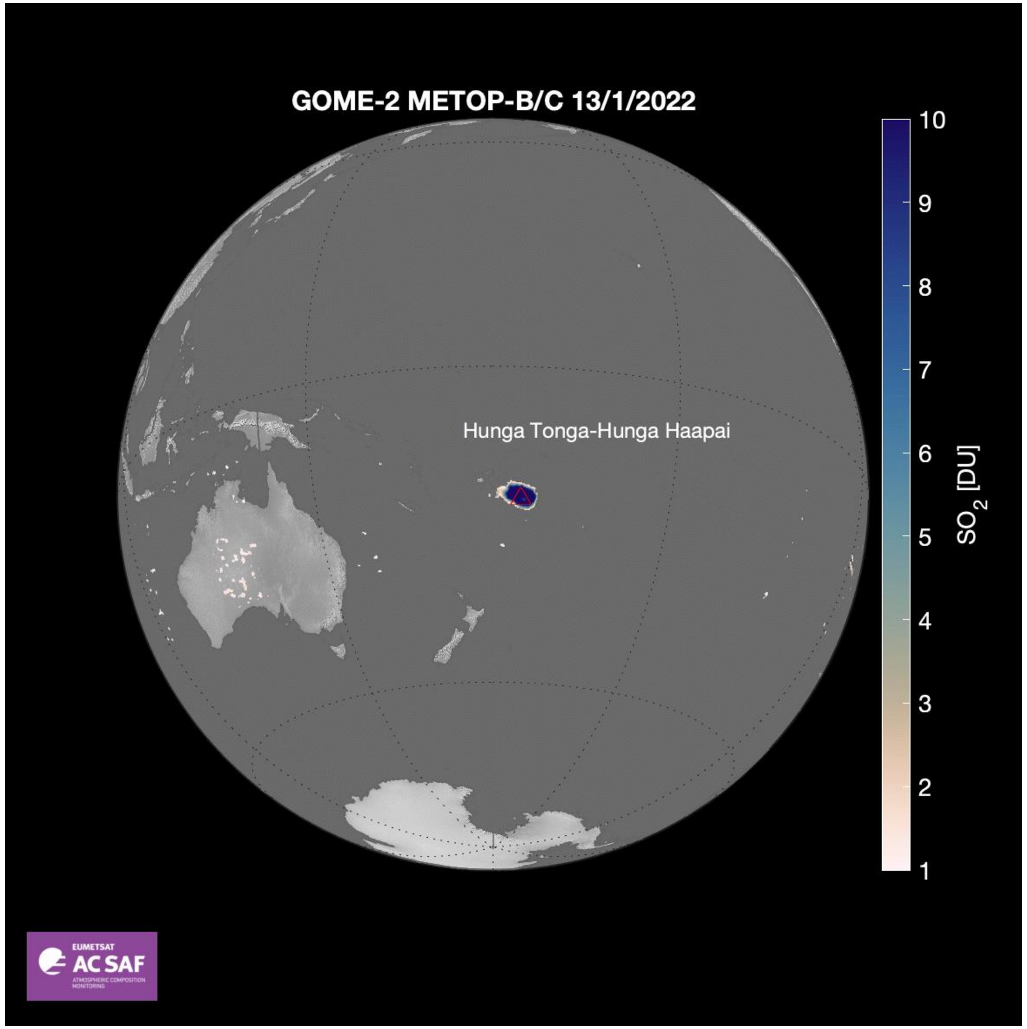
- Trace gas observing UV-VIS instruments
  - TROPOMI (Sentinel 5p)
  - OMI (Aura)
  - GOME-2 (Metop (A)/B/C)
  - OMPS (Suomi NPP)
  - GEMS (geostat.)

- Coming missions
  - Sentinel 5
  - Sentinel 4 (geostat.)
  - Tempo (geostat.)



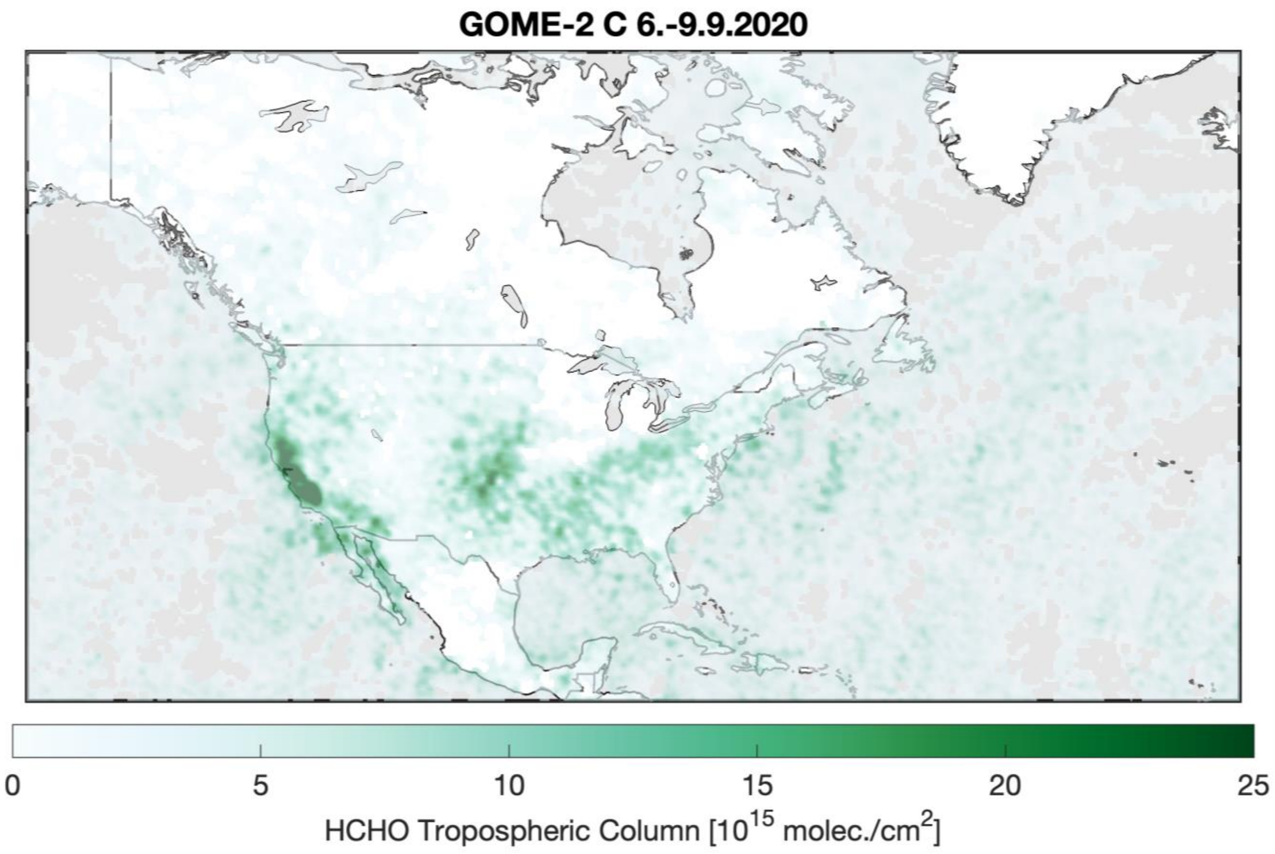
Example: Hunga Tonga eruption in Jan 2022

SO_2 from GOME-2 B&C instruments



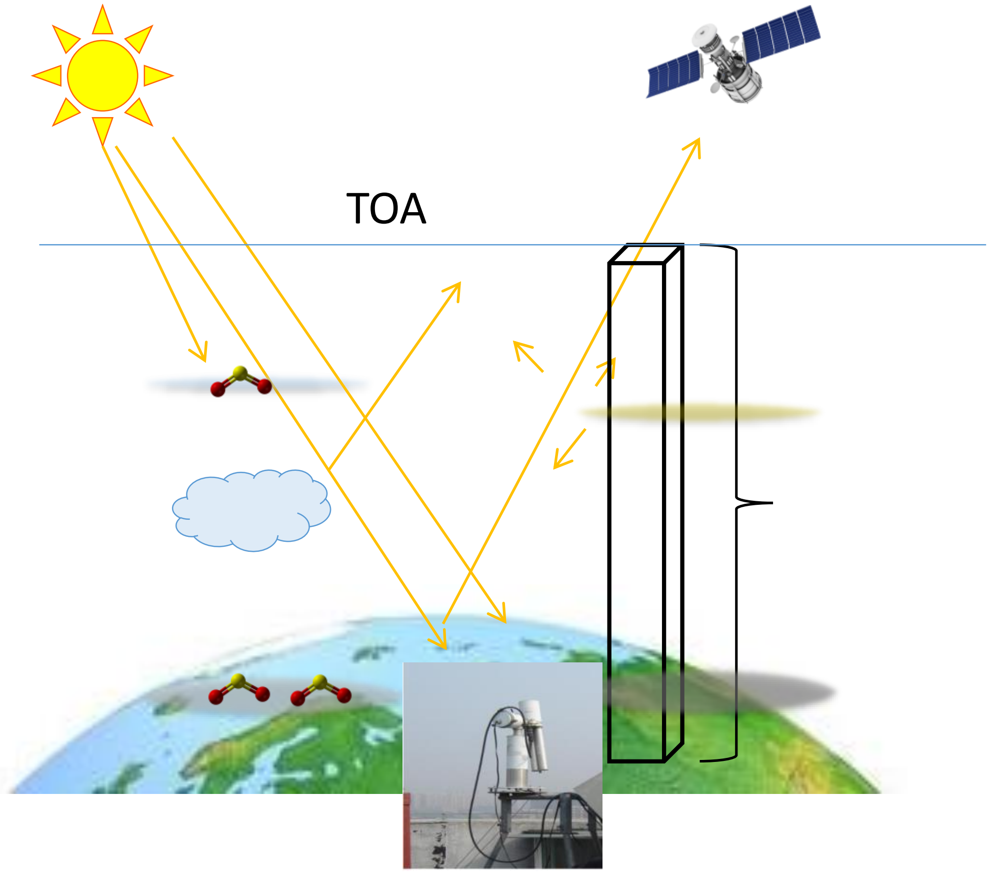
Enhancement of formaldehyde due to California fires in Sept. 2020

EUMETSAT
AC SAF
ATMOSPHERIC COMPOSITION MONITORING



Validation

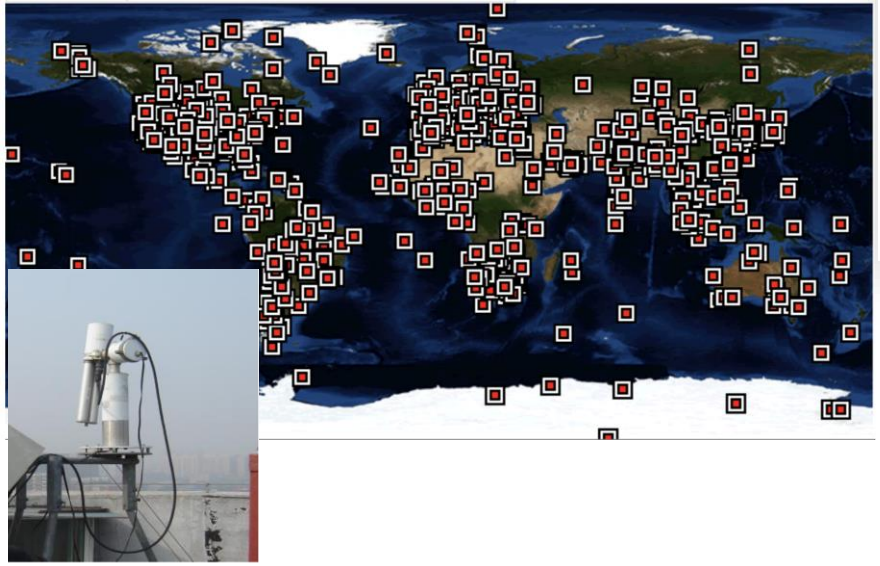
- Validation of satellite observations is essential, also for retrieval algorithm development.
- Most of the satellite parameters are validated using ground-based remote sensing networks.
- validation of satellite remote sensing measurements is a major task and often not possible in a “strict sense”
  - Spatial, temporal collocation etc.
  - AAI is a “special case” of L2 products, no ground-based validation available
- Validation should be carried out in various environments to obtain comprehensive information on algorithm performance
- L2 satellite data contains important information on (pixel level) uncertainties and quality assurance
  - **When using satellite data it is very important to follow the guidelines given by algorithm science teams!**



Examples of Ground-based remote sensing networks used for satellite observation validation

AERONET

https://aeronet.gsfc.nasa.gov/



Pandonia Global Network

https://www.pandonia-global-network.org/home/documents/

TCCON

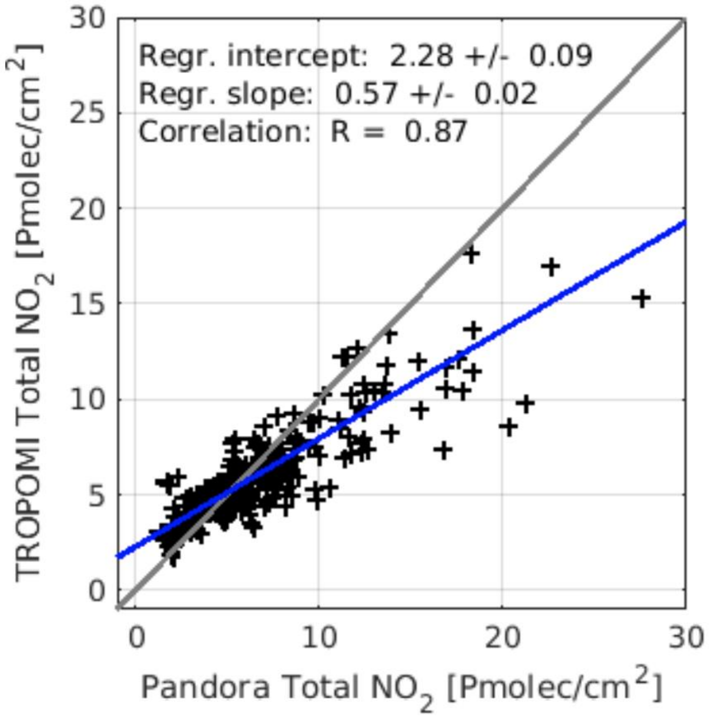
Total Carbon Column Observing Network

https://tccondata.org/

Examples of validation

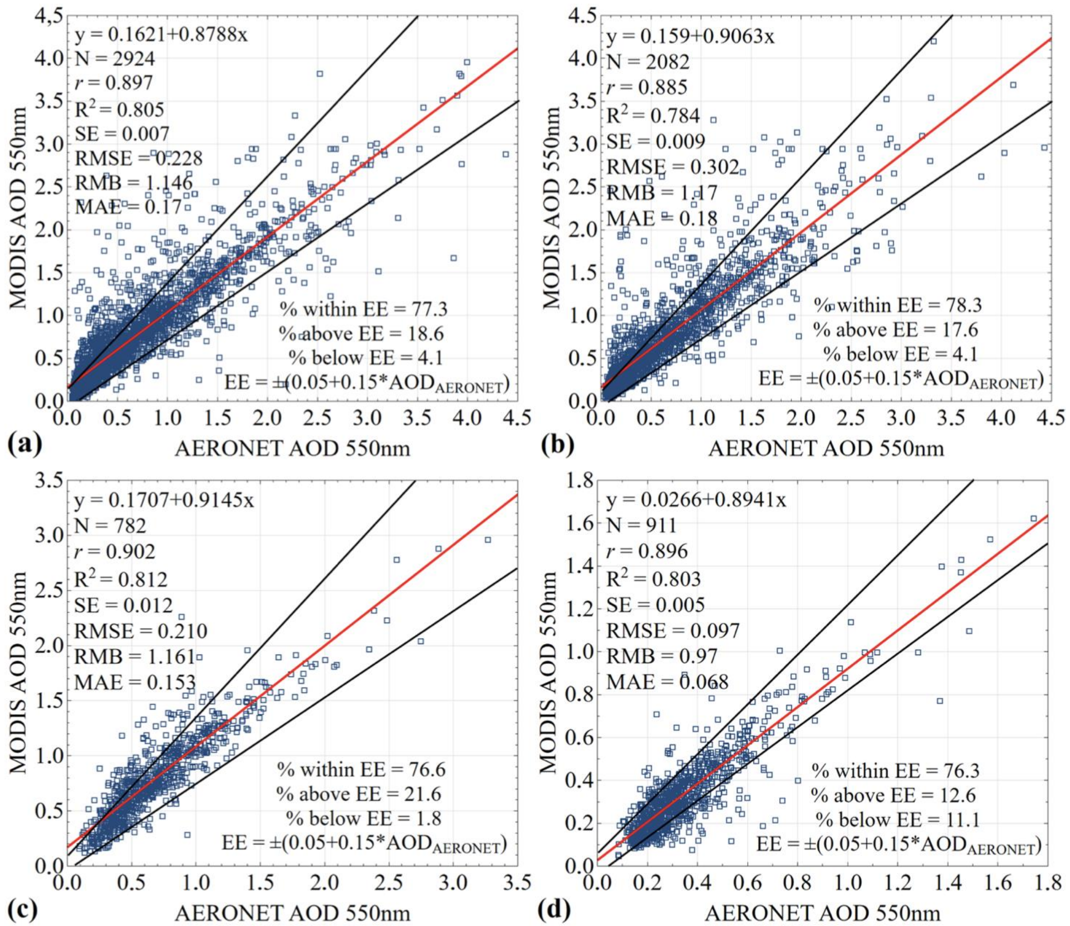
TROPOMI total NO_2 vs. ground-based Pandora total NO_2

Boulder, Colorado



Verhoelst et al., 2021

MODIS AOD vs. AERONET AOD



Filonchyk et al., 2019

Summary

- Satellite remote sensing in an indirect observation method, for atmospheric observations the key is the fingerprint that the constituent leaves to the radiation.
- Despite the differences in the approaches/wavelengths used in the algorithms, common features can be summarized as:
  - The input is L1b data (calibrated radiation measurements)
  - Most of the retrieval algorithms require the use of a priori information, which has an impact on the results
  - Spectral fitting of modelled and measured data
  - End product: L2 data, in addition to the retrieved parameters contains important information on e.g. parameter uncertainty and quality assurance

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