Activities at Max Planck Institute for Chemistry for Sentinel 4

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- Specific challenges of verification activities for S4
- Products and involved institutions
- Generation of test data sets (TDS)

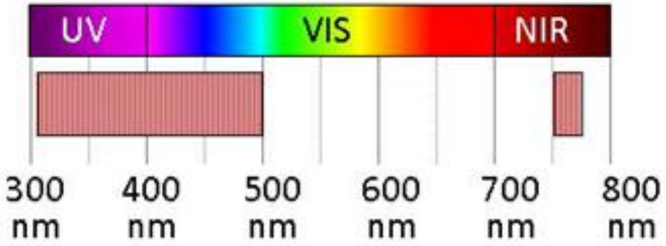
(In cooperation with S4 team)

Sentinel 4/UVN Instrument

- Geostationary satellite monitoring Europe
- MTG-Sounder (MTG-S) satellite
- 2D hyperspectral detector
- Resolution: 0.5 nm (UV-VIS), 0.12 nm (NIR)
- Spectral range:

Stark, ESA

Band	UV	VIS	NIR
Spectral range [nm]	305-400	400-500	750-775



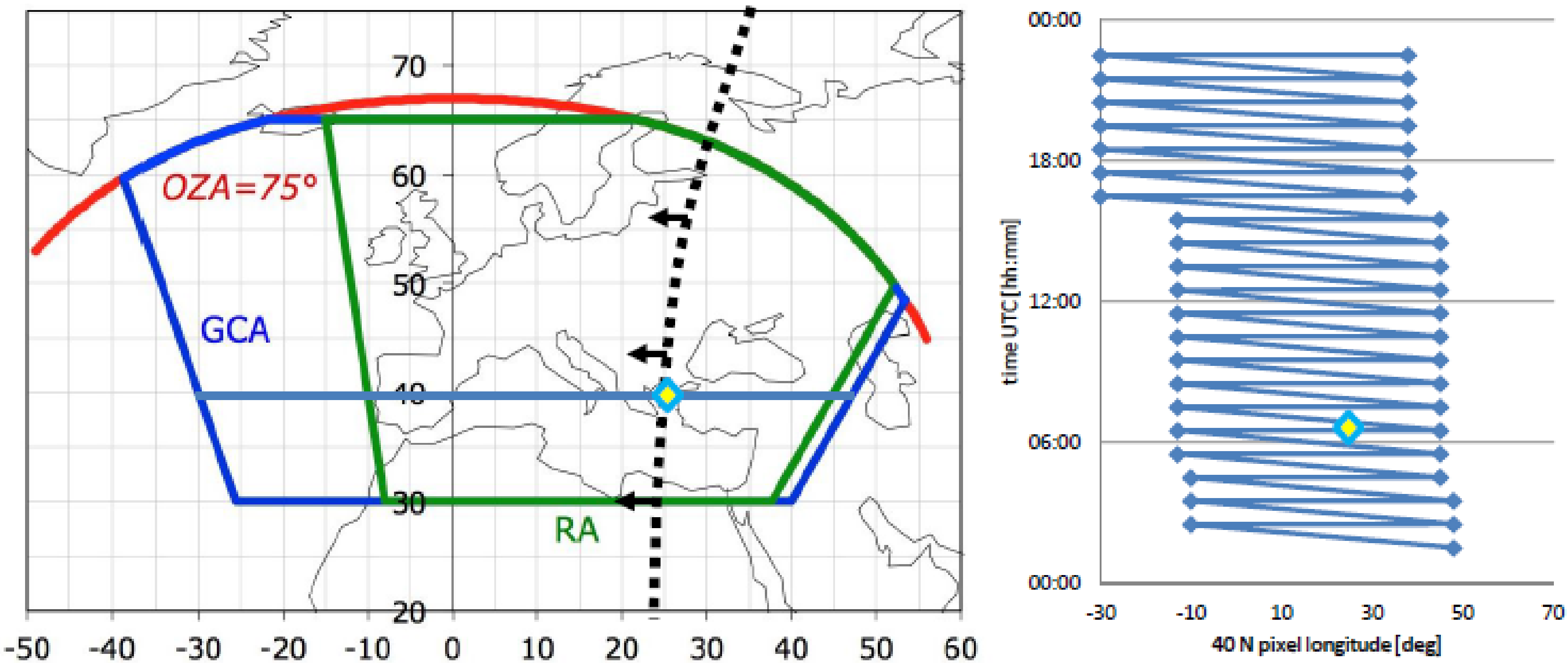
Stark, ESA

- Launch planed in 2021

S4 scanning and data acquisition

GCA = Geographic Coverage Area
RA = Reference Area
IFOV = Instantaneous Field Of View

OZA = observation zenith angle



- SSD ~8 km in E/W and in N/S at ref point (45N lat, lon of SSP)
- Angular sampling grid ~evenly spaced in Field Angle and Scan Angle
- SSD varies spatially across GCA with distance sat-target and VZA at target

Graphic & text adapted from Ben Veihelmann, ESA

Specific challenges of the S4 mission

Because S4 is ESA‘s first geostationary atmospheric chemistry mission, no measurement data with the same properties can be used.

➢ Verification activities focus on synthetic data!

Diurnal and seasonal variations of atmospheric properties have to be covered:

- trace gases
- Aerosols
- clouds

Realistic surface reflectance data (BRF) have to be considered

Specific challenges of the S4 mission

ESA's first geostationary atmospheric composition mission

- ➢ the simulation and interpretation of the atmospheric radiative transfer is different compared to previous missions in many respects:
- The same ground scenes will be observed under varying solar illumination conditions (SZA and relative azimuth angle) during the course of the day (and also for different seasons).
- BRF-Effects (for trace gas, but also for cloud and aerosol products) have to be considered
- Limited spatial coverage: new ‚reference regions' and reference techniques have to be found for trace gas retrievals (e.g. to estimate stratospheric NO2)

Level-2 Processor Development Consortium lead by DLR

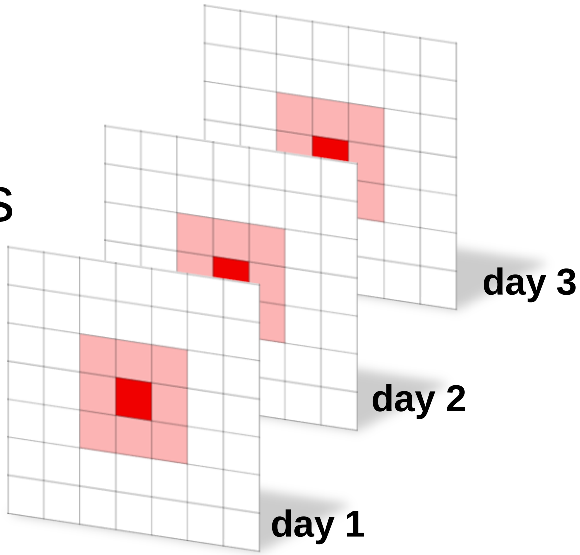
Product Processor	Algorithm Bread-boarding lead by RAL	Independent Verification lead by MPIC	Processor Suite lead by DLR
O_3 total col	DLR/BIRA	KNMI	DLR
O_3 tropospheric col	RAL	KNMI	RAL
NO_2 total & tropospheric col	IUP-UB/KNMI	MPIC/DLR	DLR
HCHO total col	BIRA/IUP-UB	IUP-UB/BIRA	DLR
SO_2 total col	BIRA	MPIC/DLR	DLR
CHOCHO (TBC)	IUP-UB/BIRA	BIRA/IUP-UB	DLR
Aerosol (Layer Height & Index)	KNMI	RAL/MPIC	KNMI/S&T
Surface and AOT	LOA/Catalysts	Rayference/Catalysts	Catalysts
Clouds	DLR	IUP-UB	DLR

- Simulation of Synthetic spectra (Test Data Set) at MPIC

Generation of synthetic spectra

Approach 1: Set of selected locations

- full diurnal cycle of three consecutive days both for June and December 2003
- the focus of this approach is to represent ***temporal variability*** over the day
- 3x3 pixel area around selected S4 pixel



Selected pixel
3x3 area around
S4 pixel grid

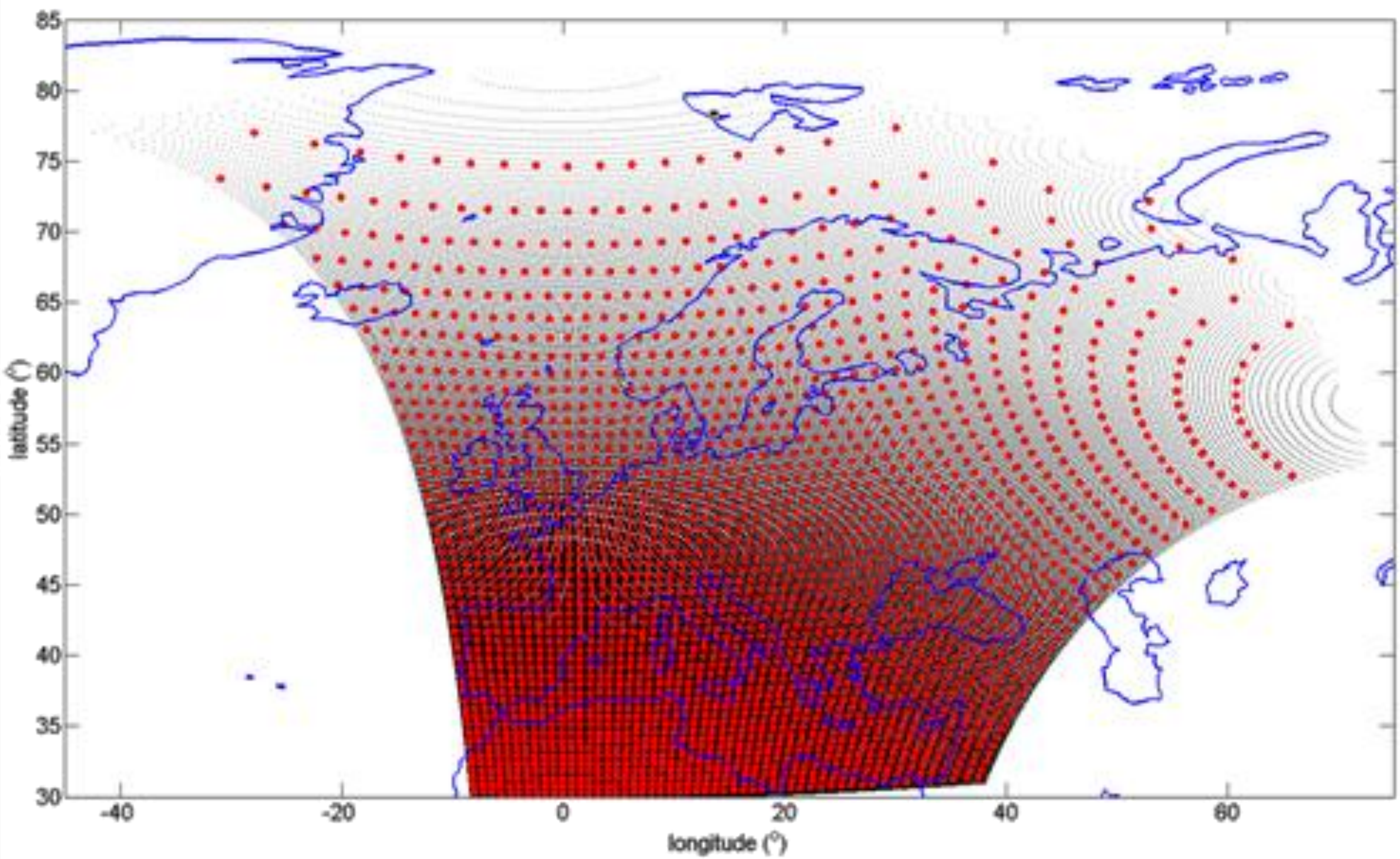
Approach 2: whole S4 area

- two days in June and December 2003.
- the focus of this approach is to cover the ***spatial variability***.
- only for every 100th S4 pixel a full spectrum will be calculated (by selecting every 10th pixel in each direction)

Selected Pixel Approach 1

Location	Latitude	Longitude	Specific properties
Helsinki	60.17°N	24.93°E	high latitude
Moscow	55.75°N	37.62°E	high latitude (winter), east side of the S4 area
Copenhagen	55.68N	12.51E	High latitude, full seasonal coverage
North Atlantic	55°N	345°E	(south-east of Iceland), north-west side of the S4 area
Cabauw	51.98°N	4.93°E	high NO_2, relatively low aerosols
Milano	45.47°N	9.18°E	high NO_2, high HCHO, high aerosols
Atlantic	46°N	357°E	(west of France) ocean, clean air
English Channel	50.20°N	0°E	ocean, polluted air
Desert	32°N	2°E	desert, low latitude
Cairo	30.05N	31.23E	south-west part of S4 area
Rabat	33.97N	-6.83W	south-east part of S4 area
Kaiserslautern	49.35N	7.85E	forest
North-East Germany	53.92°N	12.75°E	rural background station over land
Benkovski	42.42N	25.92E	farm land
Paris	48.85°N	2.35°E	urban surface
Madrid	40.42°N	356.3°E	high altitude
Bolzano	46.5°N	11.35°E	surrounded by high mountains

Approach 2



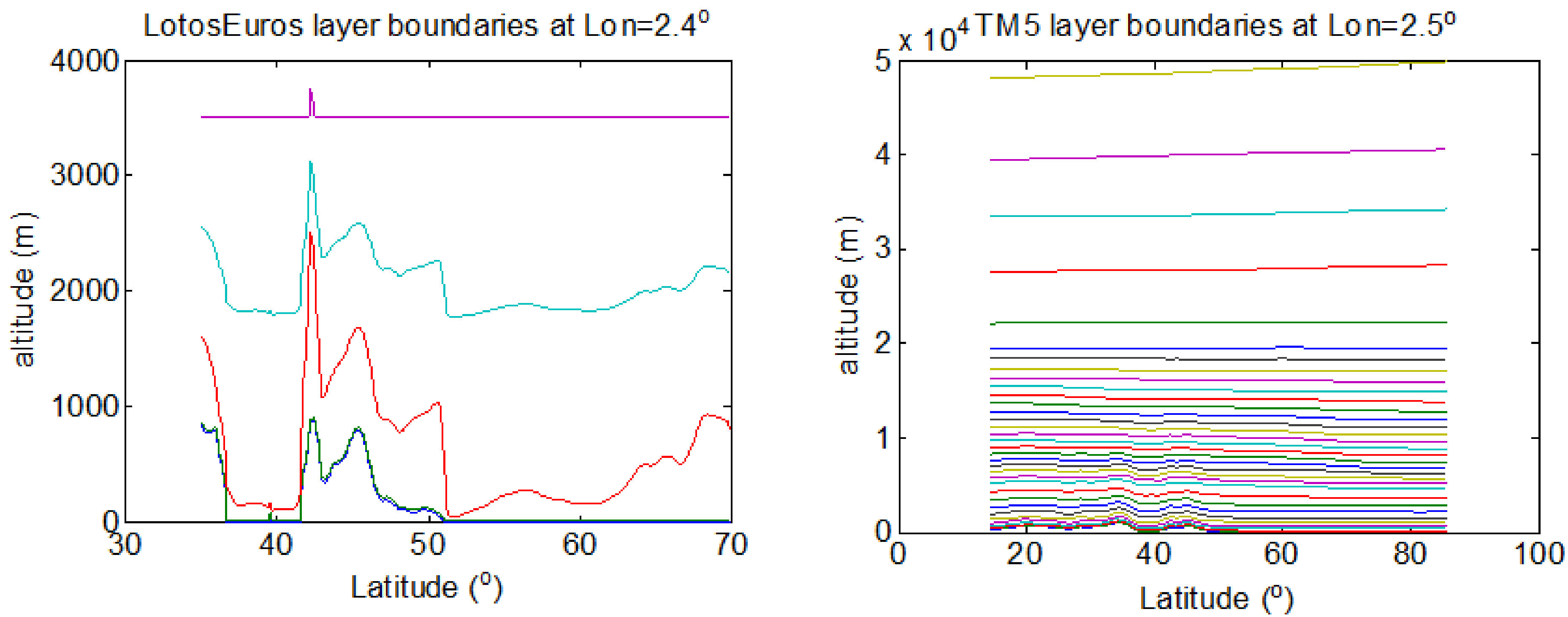
Example for the sampling of the full S4 scan for approach 2.

Input into simulations

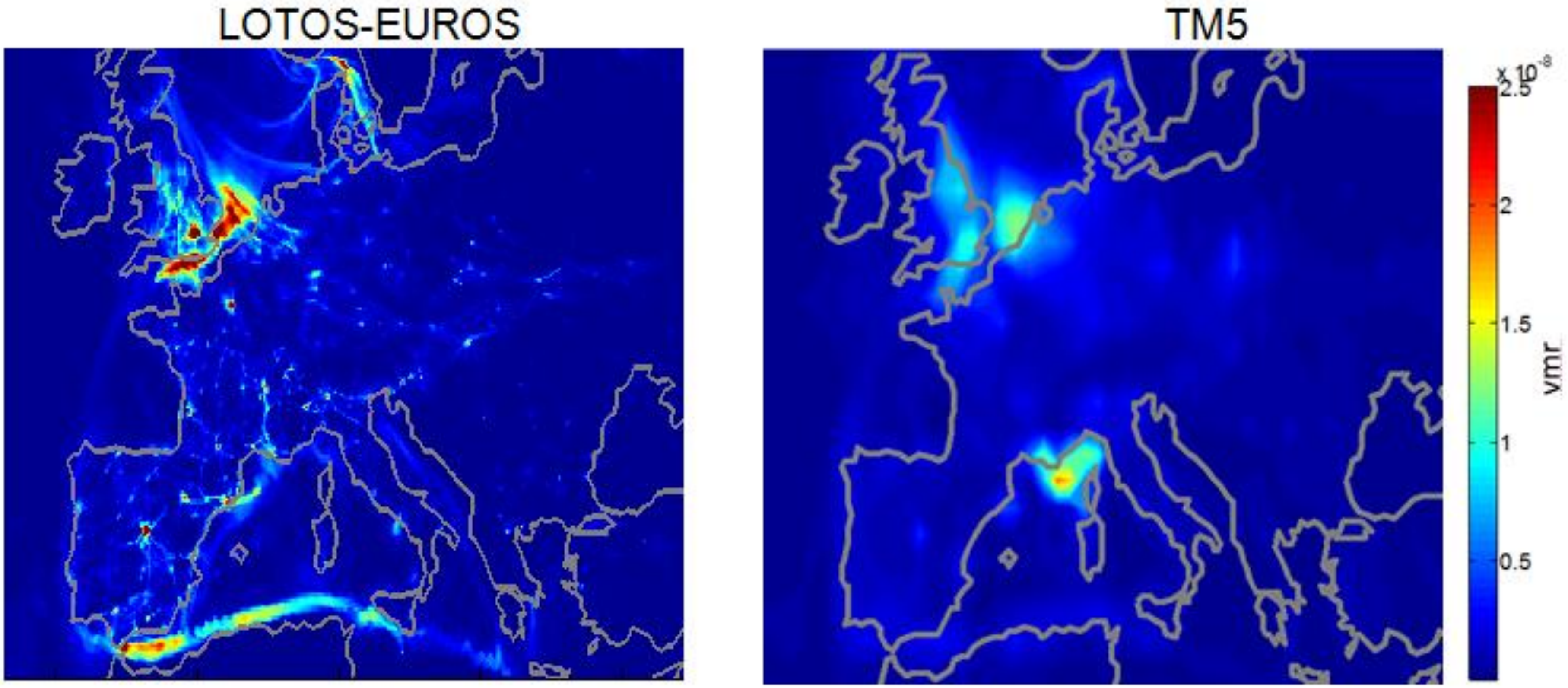
1) **NO_2, HCHO and O_3**: Diurnal variations of trace gas concentration profiles are taken from model simulations:

- 0 to 3.5km: Lotos-EUROS, high spatial resolution (MACC domain (15°W-35°E, 35°N-70°N) with about 7 km horizontal resolution)
- above 3.5km and outside MACC domain: TM5, lower spatial resolution (1°x1°, covering the area from 80°W to 85°E and 14°N to 86°N)
  (model data from Isotrop project, Henk Eskes pers. comm.)

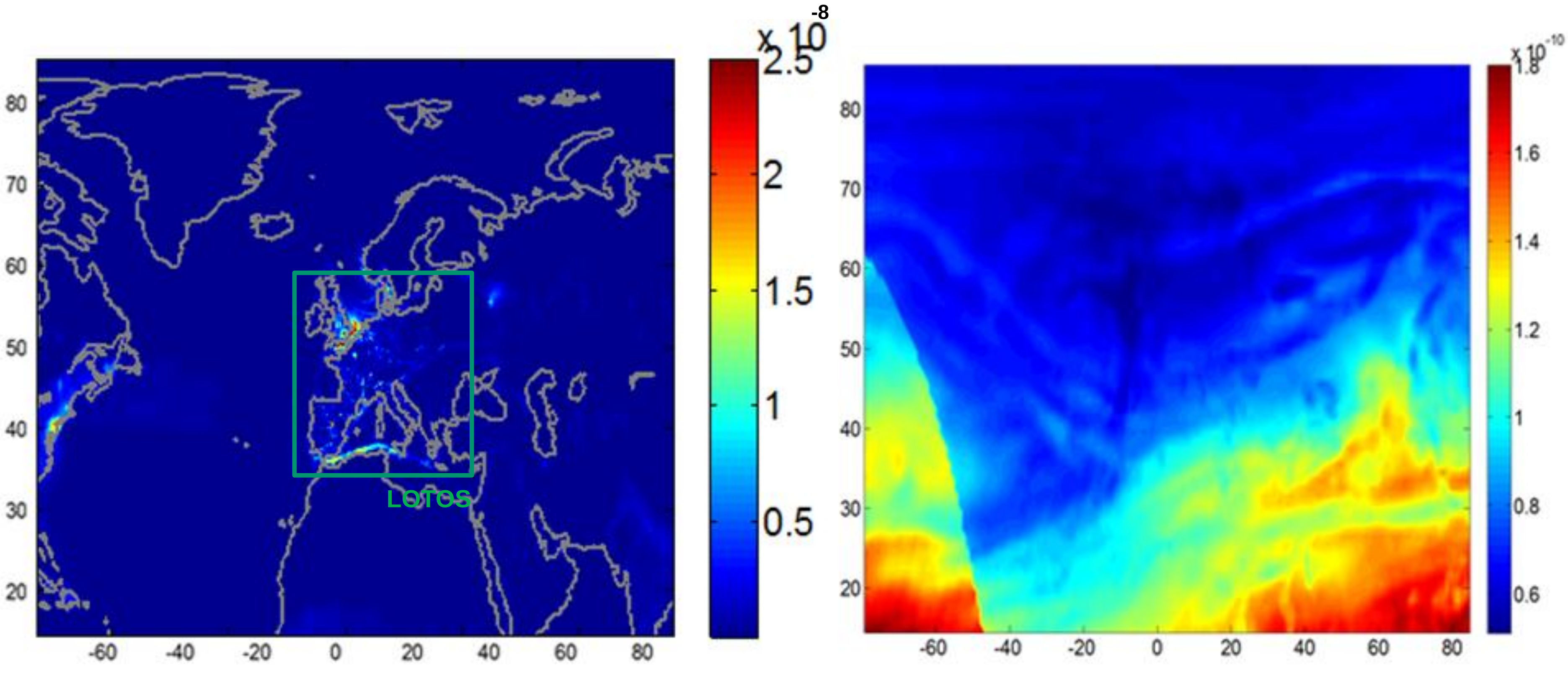
2) **SO_2**: prescribed scenarios for Boundary layer pollution and volcanic emissions are used



Variation of the vertical grid of the LOTOS-EUROS model (left) and the TM5 model (right) as function of the latitude for a longitude around 2.5°. The lines at the lowest altitude indicate the surface elevation (data for 01 June 2003, 9:00 UTC).



NO_2 surface mixing ratio over Europe from LOTOS-EUROS (left) and TM5 (right). (data for 01 June 2003, 9:00 UTC).

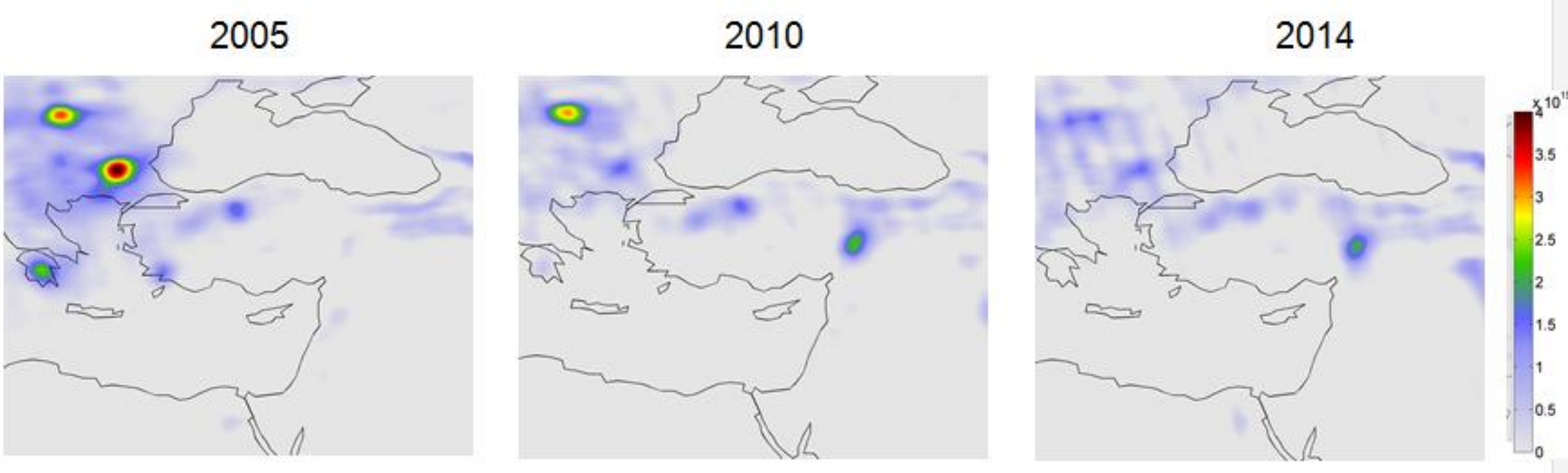


NO_2 mixing ratios at different altitudes. Left: Surface mixing ratio from combined LOTOS-EUROS and TM5 model data. Right mixing ratio at ~24.5km altitude from TM5. (data for 01 June 2003, 9:00 UTC). The sharp gradient in the west is caused by the terminator.

SO_2:

A) pollution scenarios:

Two SO_2 VCDs will be used, representing low ($1 \cdot 10^{16}$ molec/cm^2) and moderate ($5 \cdot 10^{16}$ molec/cm^2) pollution levels. In recent years SO_2 over Europe has decreased significantly



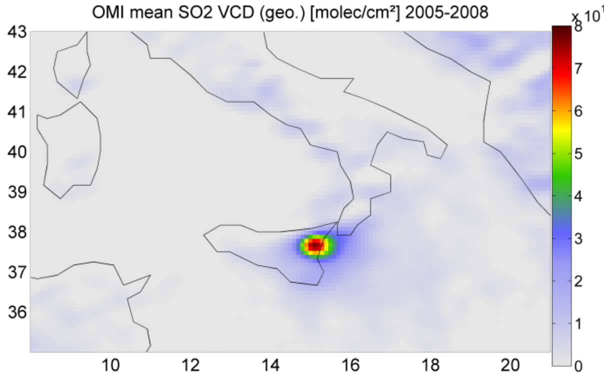
SO_2 VCDs over the middle east derived from OMI observations (Christoph Hörmann, MPIC). The VCDs were determined using a geometric AMF. Thus the true SO_2 VCDs are probably by a factor 2 to 4 larger.

B) Volcanic eruptions and degassing

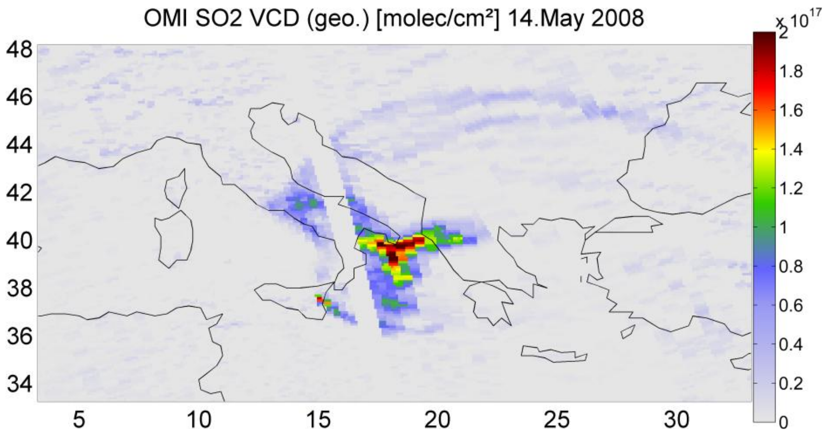
Plumes will be simulated for two scenarios:

- emissions from continuously degassing volcanoes:
  - moderate SO_2 VCD ($1 \cdot 10^{17}$ molec/cm²)
  - in a layer between 2 and 3 km.
- volcanic eruptions:
  - moderate SO_2 VCD($1 \cdot 10^{17}$ molec/cm²)
  - high SO_2 VCD ($1 \cdot 10^{19}$ molec/cm²)
  - in a layer between 8 and 9 km.

(These settings match those used within S5P verification)



C. Hörmann, MPIC

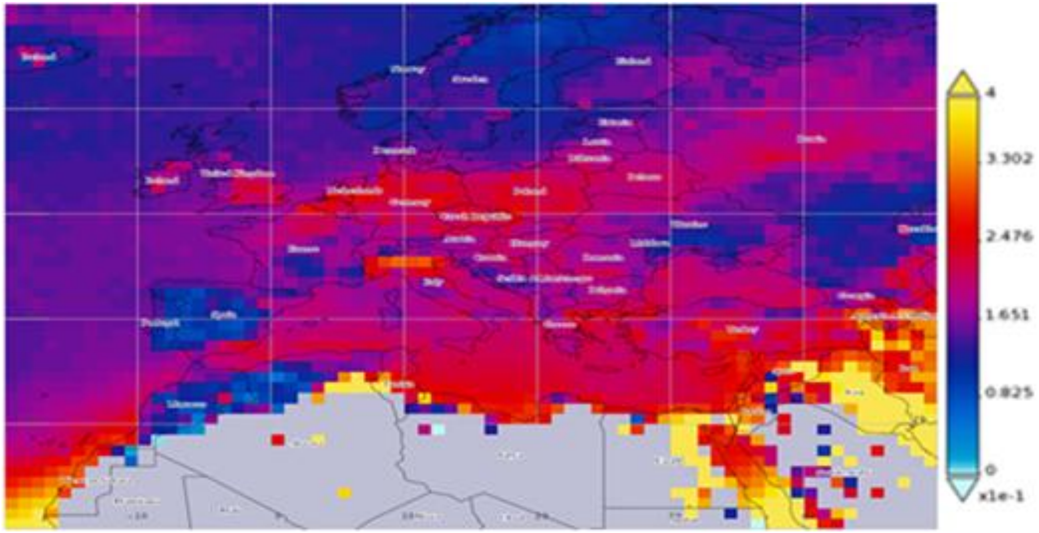


C. Hörmann, MPIC

3) Aerosols:

- AOD is taken from average MODIS observations (see below); in addition to these values also the half and double values are used.
- Angstrom parameter is set to 1
- the profile height is taken from the model data (boundary layer height)
- for desert dust aerosols an elevated aerosol layer between 3 and 4 km altitude with an AOD of 1 is assumed

Location	AOD
Helsinki	0.14
Moscow	0.23
Copenhagen	0.18
North Atlantic	0.14
Cabauw	0.26
Milano	0.32
Atlantic	0.17
English Channel	0.17
Desert	0.11
Cairo	0.41
Rabat	0.12
Kaiserslautern	0.19
North-East Germany	0.22
Benkovski	0.20
Paris	0.22
Madrid	0.13
Bolzano	0.16



Average AOD at 550 nm derived from MODIS observations (2003-2016).

© Giovanni online data system, developed and maintained by the NASA GES DISC)

4) Clouds:

- typical cloud scenarios (clear, partly cloudy, totally overcast) will be assumed
- cloud heights: 1-2km, 3-4 km, and 7-8km
- cloud OD: 5 and 20
- the independent pixel approximation (IPA) will be used

5) Temperature and pressure profiles

- taken from the TM5 model

6) Surface BRF data

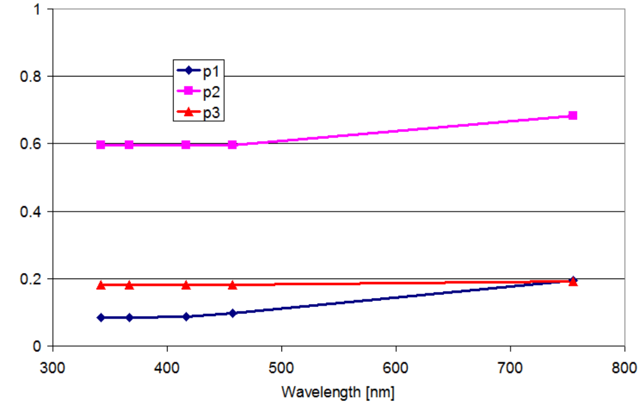
- Surface BRF data from the GRASP algorithm
- on land: BRF kernels are based on the Ross-Li parameterisation (3 kernels obtained from POLDER observations)
- over ocean: Cox-Munk parameterisation

7) Surface elevation

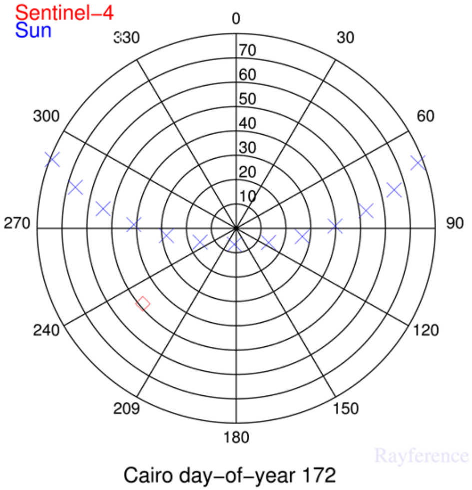
➢ To be consistent with the model data surface elevation is taken from the model data LOTOS-EUROS & TM5

BRF parameters for a selected site (Cairo)

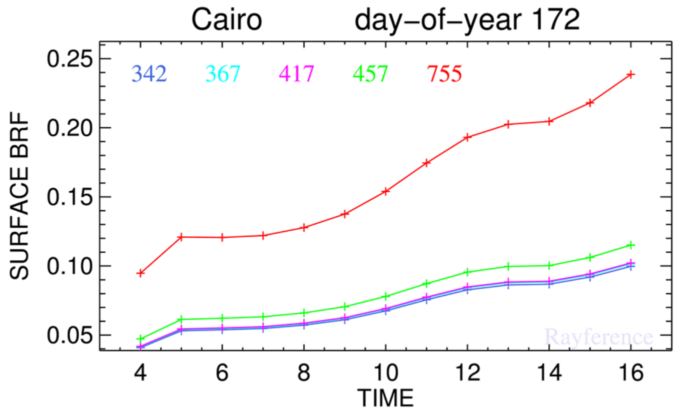
MODIS image of Cairo; the red polygon indicates the S4 ground pixel.



BRF kernels from the Ross-Li parameterisation for Cairo in Summer as function of the wavelength.



Geometries of observation (red) and illumination (blue) over the Cairo site in summer.



Surface BRF simulated over the Cairo site with the Ross-Li model in the 5 selected wavelengths.

Generation of test data sets (TDS)

- **High resolution spectra**:

  They will be provided to ESA as input to S4/UVN instrument simulations and for the calculation of synthetic L1b data. High resolution spectra will also be provided to project partners for specific tasks, e.g. to investigate the effect of heterogenous scenes on the L1b spectra.

- **S4 spectra**: spectral resolution (L1b) of the S4 instrument.

  They are derived from high resolution spectra by convolution and resampling according to the spectral properties of the S4 instrument.

  Noise will be calculated based on the simulated radiance and the instrumental properties

Simulation details:

- Simulations performed with SCIATRAN RTM
- Viewing geometry (SZA, VZA, rAA) according to time and location of selected ground pixel
- BRF according to time and location of selected ground pixel
- profiles of trace gases, aerosols and clouds are taken from model simulations or prescribed scenarios

Trace gas cross sections:

UV/VIS :	NO2, HCHO, O3, H2O, O4, SO2
NIR:	O2, H2O

- Rotational Raman is considered*
- polarisation is considered*

Sampling and resolution UV/VIS:

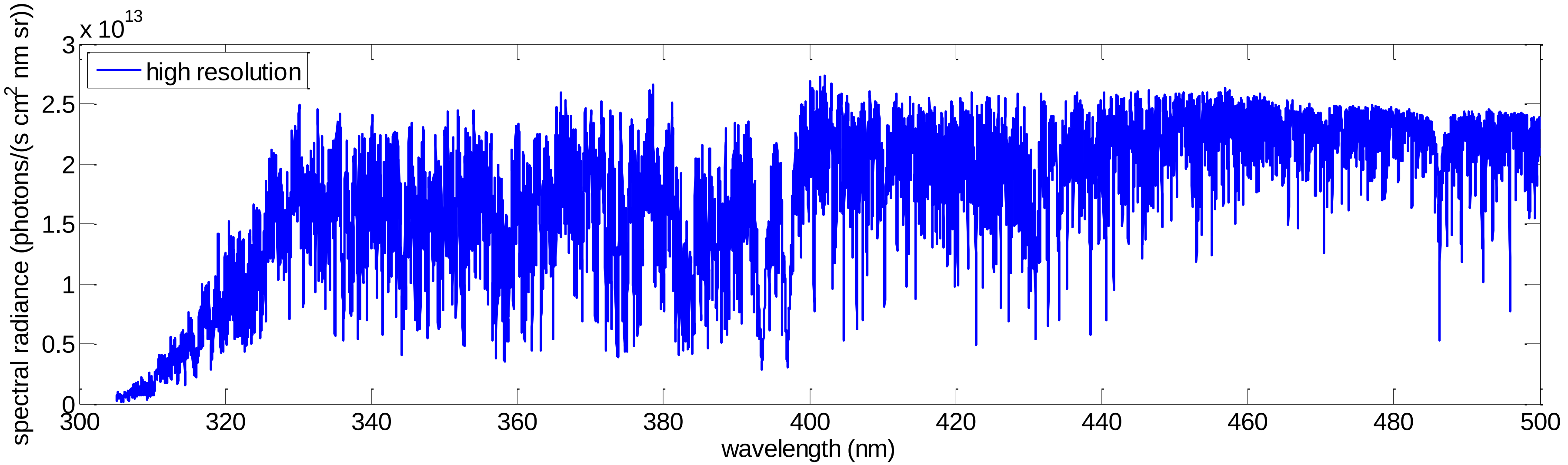
- high Resolution spectra: sampling: 0.01 nm, resolution: 0.04 nm
- low resolution spectra: sampling: ~0.16 nm, resolution: 0.5 nm

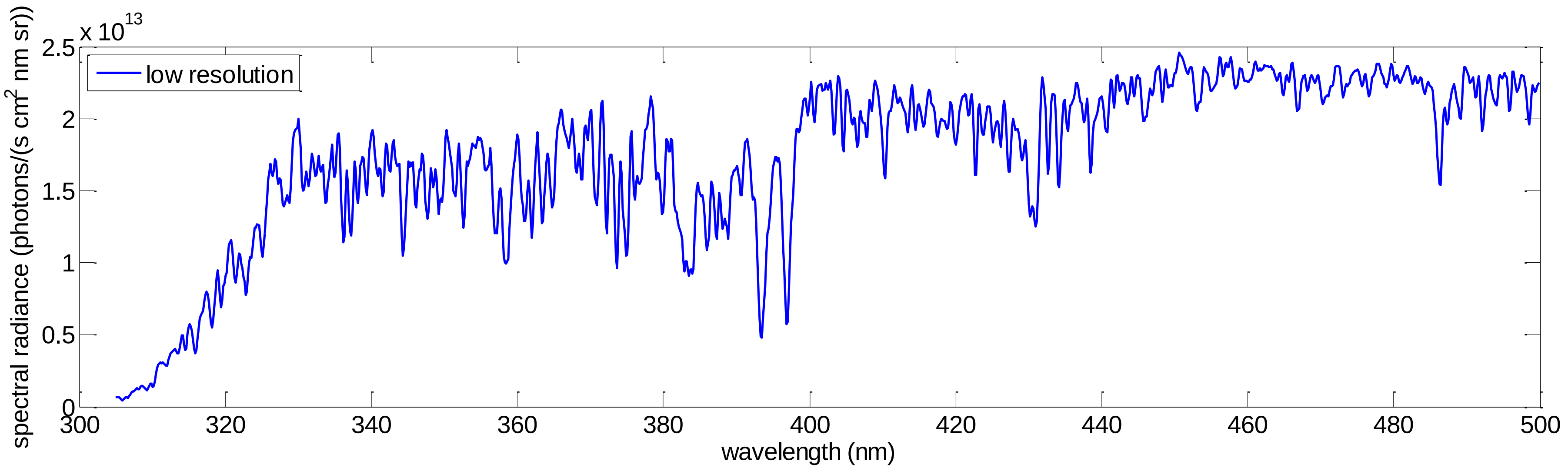
Sampling and resolution NIR :

- high resolution spectra: sampling 0.001 nm
- low resolution spectra: sampling: ~0.04 nm, resolution: 0.12 nm

*first data set without polarisation and Raman scattering

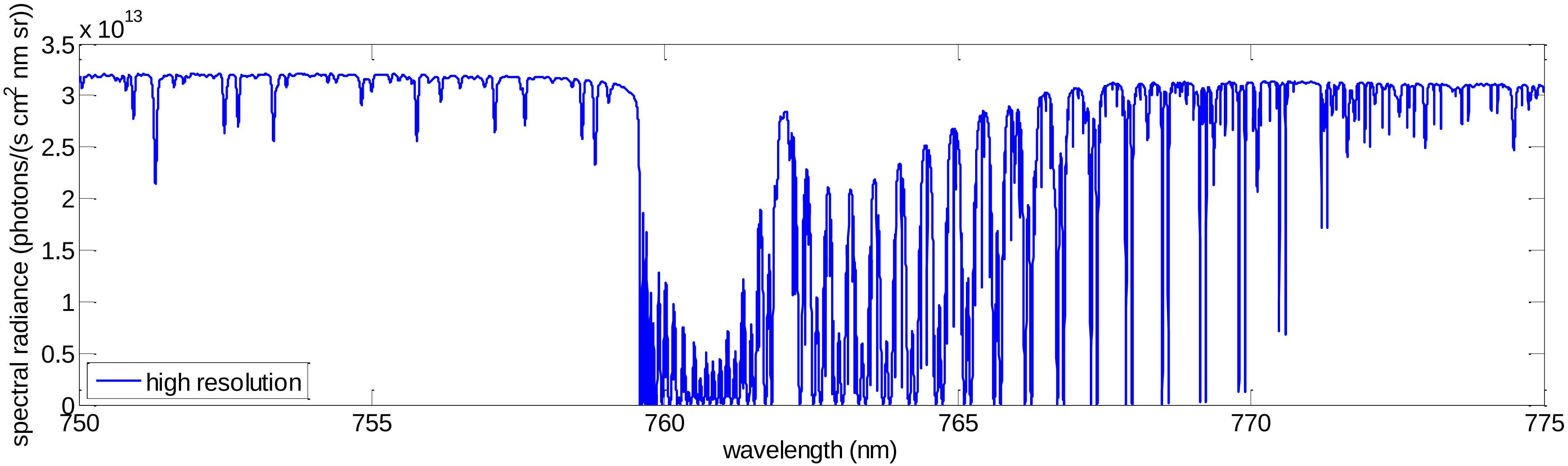
Examples of UV/VIS high and low resolution spectra

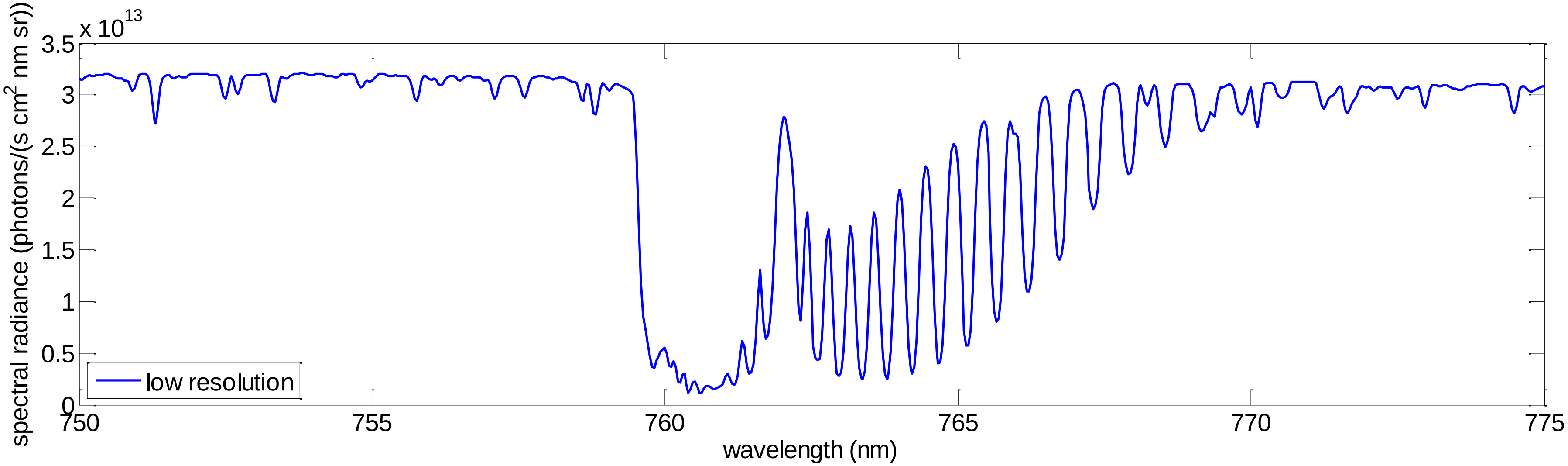




Milano (45.47°N 9.18°E, ~12:00 UTC, Raman scattering & polarization included

Examples of NIR high and low resolution spectra





Milano (45.47°N 9.18°E, ~12:00 UTC, Raman scattering & polarization included

Summary

- Verification activities are crucial for testing the operational algorithms
- For S4 (as the first geostationary chemistry mission) the verification activities are based on synthetic data
- MPIC is responsible for the definition and generation appropriate test data sets
- All relevant atmospheric scenarios and viewing geometries have to be covered
- Bidirectional reflectance properties of the surface have to be considered
- Spectra are simulated with high spectral resolution and considering polarisation and Raman scattering