3DCATS – Synthetic data: impact of 3D clouds on retrieved NO_2 VCD

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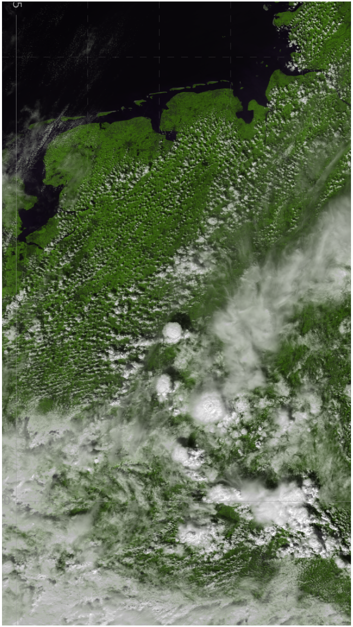
Introduction

- Operational retrievals of tropospheric trace gases from space-borne instruments based on 1D radiative transfer neglect
  1. cloud scattering into clear regions
  2. cloud shadows

- Monte Carlo radiative transfer (MYSTIC-ALIS)
  $\Rightarrow$ simulation of spectra for realistic 3D model atmospheres

- Application of NO_2 retrieval algorithm on simulated data:
  $\Rightarrow$ estimation of retrieval error due to 3D cloud scattering



Outline

- Aim: Use synthetic data to validate and improve NO_2 retrieval algorithms
- Radiative transfer model MYSTIC
  - Horizontal photon transport is essential to investigate impact of cloud scattering on trace gas retrievals ⇒ Monte Carlo RT approach
- Box cloud scenario
  - Simulated spectra and layer-AMFs
  - investigate sensitivity of NO_2 retrieval error on various parameters
- LES cloud scenario
  - Cloud scene from ICON-LES model over Europe ($698 \times 763\,km^2$)
  - All types of realistic clouds included
  - Representative sun-satellite geometries and surface albedos
  - Generate synthetic dataset for geostationary orbit and low Earth orbit for VIS and O_2A-band
  - Quantification of NO_2-retrieval error

3D radiative transfer in high spectral resolution

NO_2 retrieval (DOAS) – fit differential optical thickness

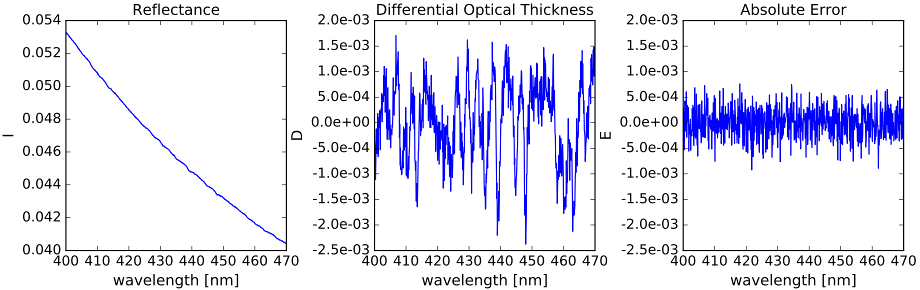
$$D(\lambda) = \ln(I_{TOA}(\lambda)) - P_3(\lambda)$$

I_{TOA}: reflectance, spectral range: $\lambda \approx$ 400-500 nm

Radiative transfer requirements:

$\Rightarrow$ high spectral resolution (resolve characteristic absorption features)

$\Rightarrow$ high accuracy (absorption signal weak compared to Rayleigh continuum)



Standard Monte Carlo method: computational time extremely high

(about 33h for 10^7 photons/wavelength and 0.1 nm spectral resolution!)

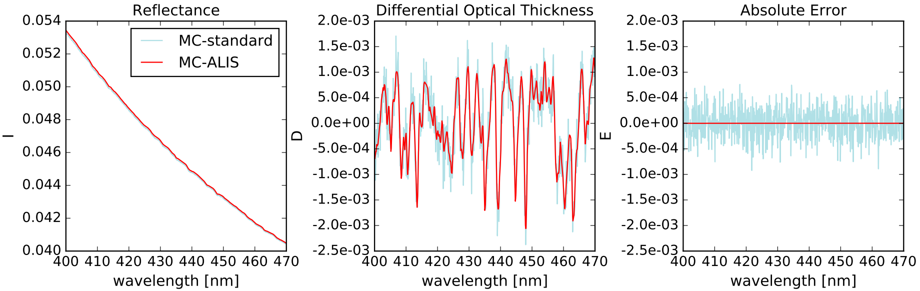
Absorption Lines Importance Sampling

Trace photons at only one wavelength and calculate full line-by-line spectra

Spectral absorption and scattering included by photon weights

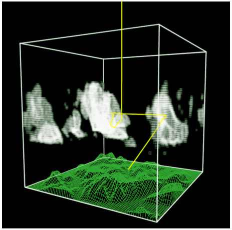
Statistical error causes bias (decreasing with $\sqrt{N}$) over full spectral range, not for each wavelength

Computational time: 1.5 minutes (comparable to DISORT)



C. Emde, R. Buras, and B. Mayer. *ALIS: An efficient method to compute high spectral resolution polarized solar radiances using the Monte Carlo approach.* JQSRT, 2011

Radiative transfer model MYSTIC

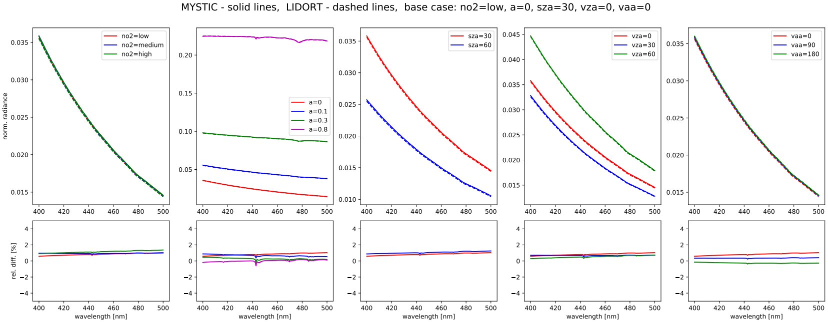


Monte carlo code for the phYSically correct Tracing of photons In Cloudy atmospheres (Mayer 2009)

- *Special features:*
    - Polarized radiative transfer (*Emde et al., 2010*)
    - VROOM: variance reduction methods (*Buras and Mayer, 2011*)
      ⇒ radiance calculations for strongly peaked scattering phase functions
    - ALIS method (*Emde et al., 2011*)
      ⇒ very efficient high spectral resolution calculations
    - complex topography (*Mayer et al., 2010*)
    - spherical geometry (*Emde and Mayer, 2007*)
    - layer/box-airmass factors in 3D domain (*Schwärzel, Emde et al. 2020*)
- Integrated in libRadtran package `www.libradtran.org` (*Mayer and Kylling, 2005, Emde et al. 2016*)

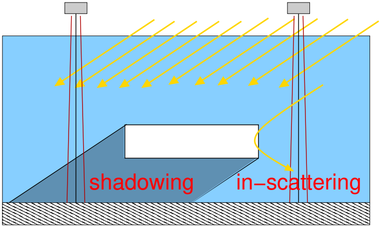
Tests in one-dimensional geometry

- Simulation of spectra in VIS (400–500 nm, 0.2 nm resolution) and O_2A-band (755–775 nm, 0.005 nm resolution)
- Model intercomparison: very good agreement between LIDORT and MYSTIC



- Application of NO_2 retrieval algorithm on synthetic spectra
  Clearsky ⇒ quantify retrieval error due to model differences
  1D cloud layer ⇒ test cloud correction schemes (O_2-O_2 and FRESCO)

Clearsky pixels in vicinity of clouds



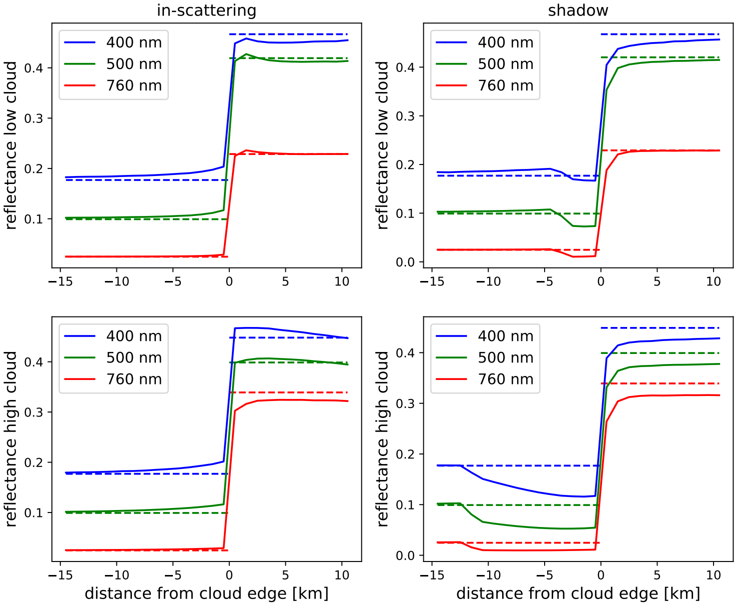
Sketch of box cloud setup.

General settings

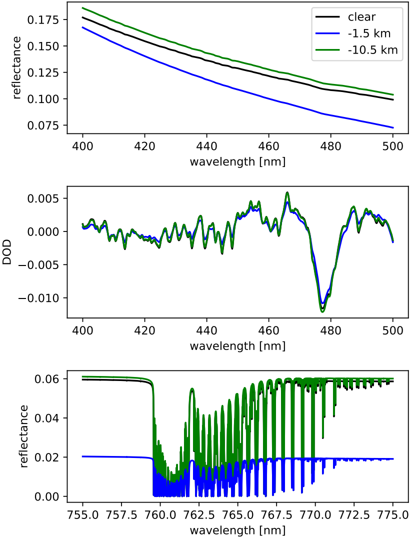
- nadir observation geometry
- 1x1km^2 square field-of-view
- NO_2 profiles: Pacific polluted, European polluted
- surface albedo: 0.05
- no aerosol

	liquid water cloud	ice water cloud
cloud optical thickness	1, 2, 5, **10**, 20	1, 2, **5**, 10, 20
cloud bottom height [km]	**2**, 5, 10	5, **9**, 12
effective radius [μm]	10	30
optical properties	Mie	Baum (V3.6)
cloud geometrical thickness [km]	0.2, **1**, 2, 4, 8	
surface albedo	0.02, **0.05**, 0.1, 0.15, 0.2, 0.3	
solar zenith angle [°]	20, 30, 40, **50**, 60, 70, 80	

Reflectance as function of distance from cloud edge

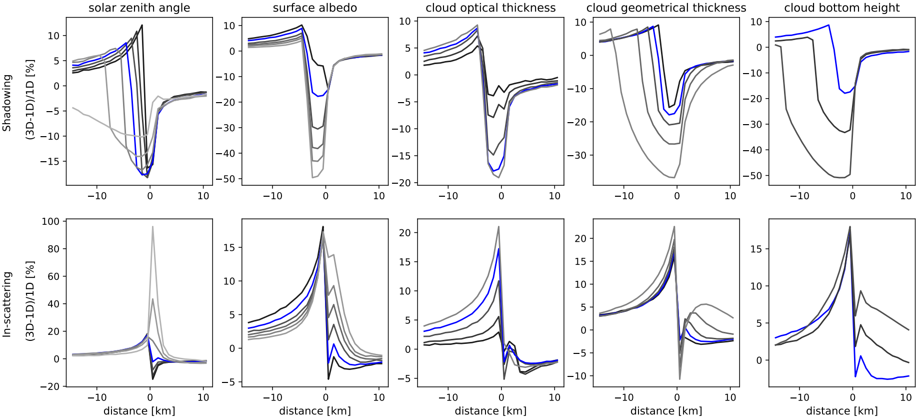


Simulated spectra in clear region



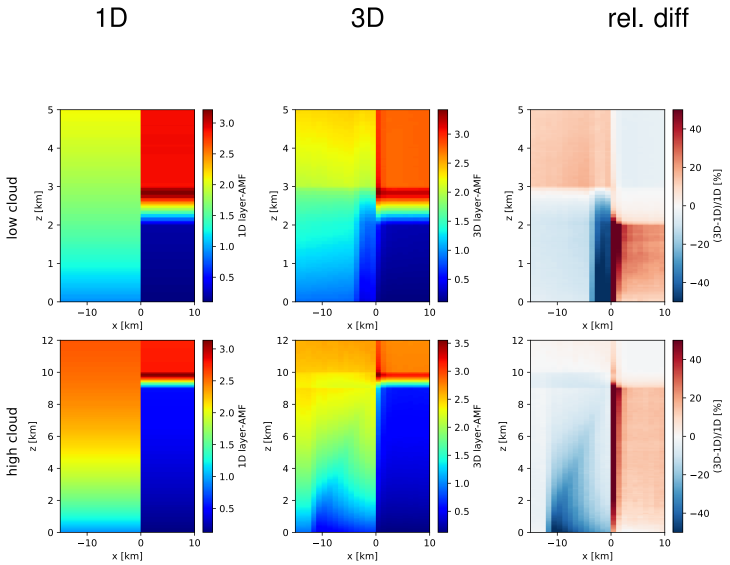
- VIS: 400–500 nm, $\Delta\lambda$=0.2 nm
- $DOD(\lambda) = \ln(I(\lambda)) - P_3(\lambda)$
- O_2A band: 755–775 nm, $\Delta\lambda$=0.005 nm

Rel. diff. between 3D and 1D reflectance (460nm)



	liquid water cloud	ice water cloud
cloud optical thickness	1, 2, 5, **10**, 20	1, 2, **5**, 10, 20
cloud bottom height [km]	**2**, 5, 10	5, **9**, 12
cloud geometrical thickness [km]	0.2, **1**, 2, 4, 8	
surface albedo	0.02, **0.05**, 0.1, 0.15, 0.2, 0.3	
solar zenith angle [°]	20, 30, 40, **50**, 60, 70, 80	

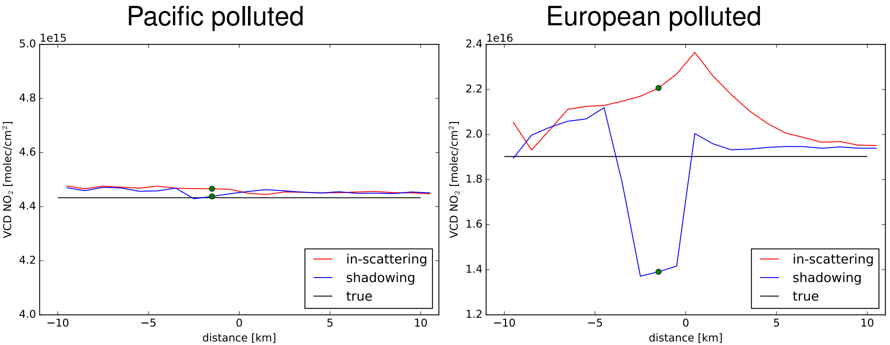
Layer-AMFs for base cases, cloud shadow



NO_2 retrieval algorithms

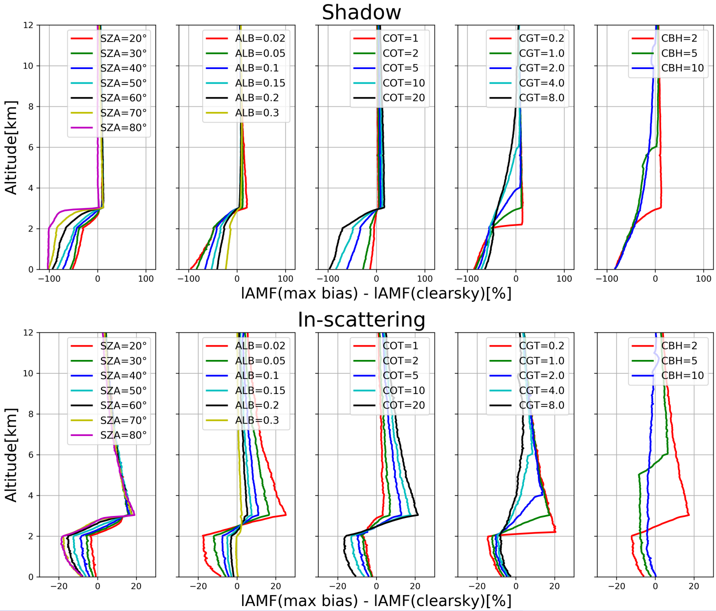
- Standard approach:
  - 1. DOAS fit is performed using the QDOAS software (Danckaert et al., 2017) ⇒ NO_2 slant column densities (SCD)
  - 2. Convert SCD to vertical columm densities (VCD) using air mass factors (AMF)
- AMF calculation: integral of the relative vertical NO_2 distribution, weighted by layer-AMF computed with a radiative transfer model (VLIDORT).
- Cloud correction uses cloud fraction, cloud top pressure and cloud top albedo from two cloud retrieval algorithms: O_2-O_2 (Acarreta et al.,2004) and FRESCO (Koelemeijer et al., 2001)

NO_2 retrieval results

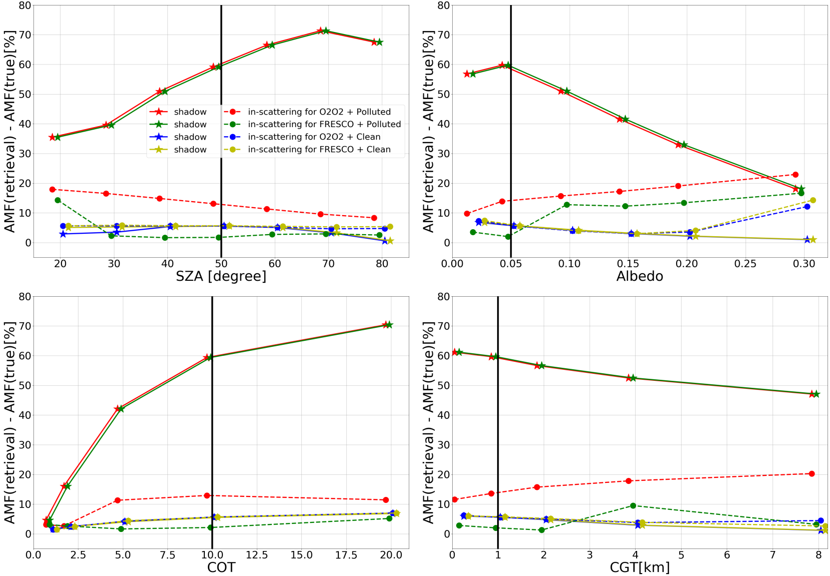


NO_2 retrieval results depending on distance from cloud edge.

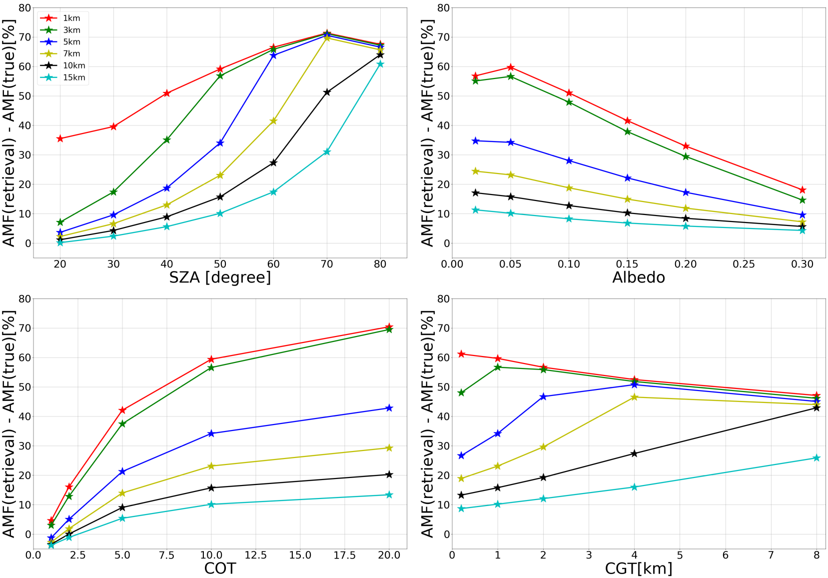
Layer-air-mass factor retrieval error



Impact of NO_2 profile



Impact of spatial resolution



Summary - sensitivity of retrieval error

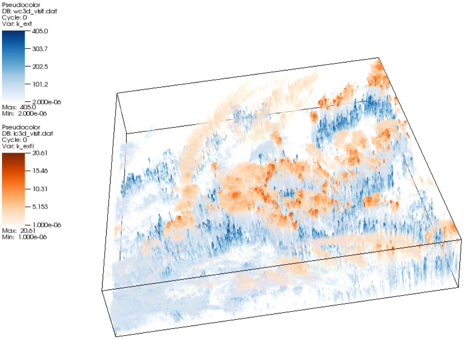
- retrieval error in cloud shadow is large
  - $\approx$35% for SZA=20° to more than 70% for SZA=80°
  - affected area extends to 1km from the cloud edge for SZA=20° to more than 15km for SZA=80°
  - 60% for low surface albedo (0.02/0.05), decreases to 10% for albedo=0.3
  - 5% for COT=1 to 70% for COT=20
- retrieval error in in-scattering region relatively small ($<$20%), affected area is within 5 km from cloud edge

LES cloud scenario

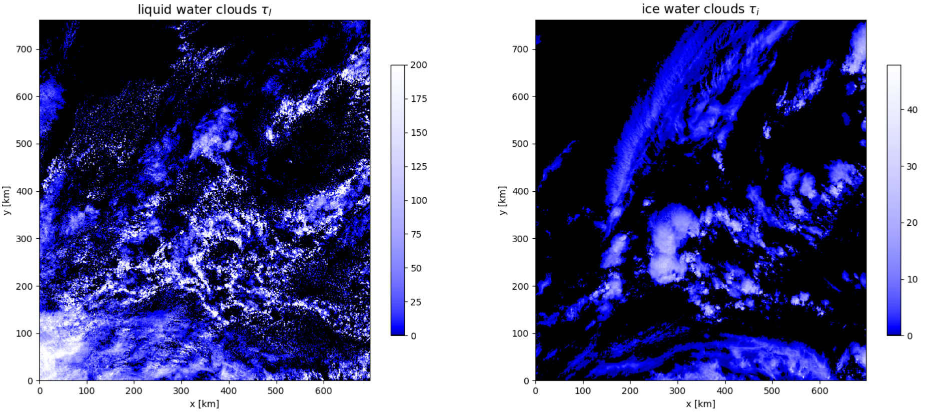
ICON model

ICOsahedral Nonhydrostatic atmosphere model;
Dipankar et al. 2015, Zängl et al. 2015

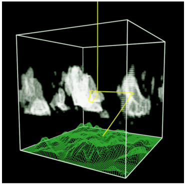
- Spatial resolution approx. 1 km for region including Germany, Netherlands and parts of other surrounding countries
- Model validated against ground-based and satellite based observational data (Heinze et al. 2017)
- Simulations include all cloud types that are typical for Europe (e.g. shallow cumulus, cirrus, stratus, and convective clouds)



Vertically integrated cloud optical thickness



Reflectance simulation with LES clouds

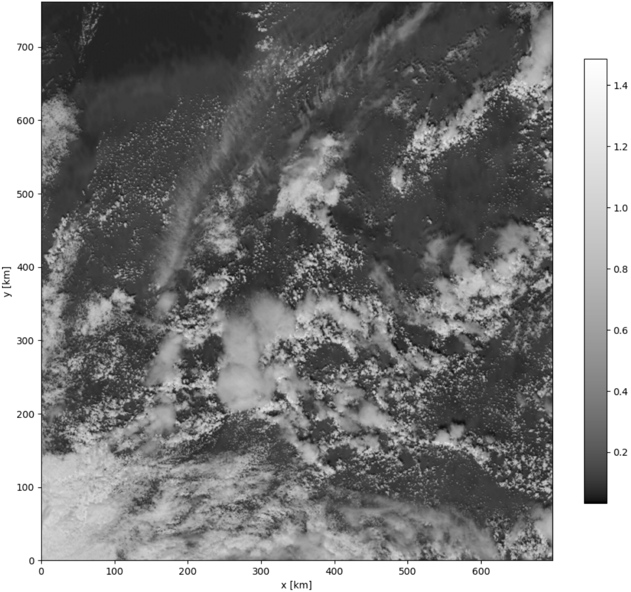


MYSTIC – Monte Carlo radiative transfer model
Mayer 2009, Emde et al. 2011, Emde et al. 2016

- Central wavelength 554 nm, Bandwidth 19.26 nm (Sentinel3 SLSTR B1)
- Nadir view, spatial resolution 1.2 km, 588×624 pixels
- Sun position SZA: 30°, SAA: 13°
- Surface albedo data from MODIS
- US standard atmosphere
- ICON clouds (3D liquid and ice water content fields)
- Effective radii parameterized following Bugliaro et al. 2011
- Optical properties:
  liquid water clouds: Mie
  ice water clouds: general habit mixture; Yang et al. 2013, Baum et al. 2014

Statistics of synthetic data can be compared to real satellite observations to verify whether clouds are realistic.

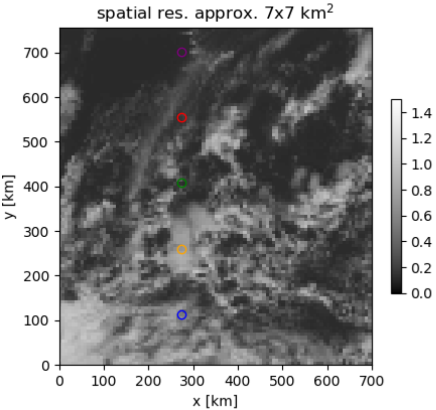
Simulated reflectance image for LES scene

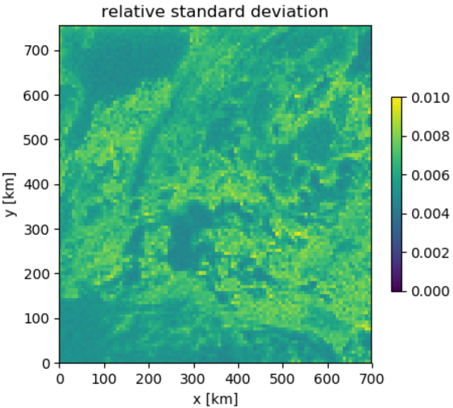


Sentinel-5 reflectance simulation for LES scene

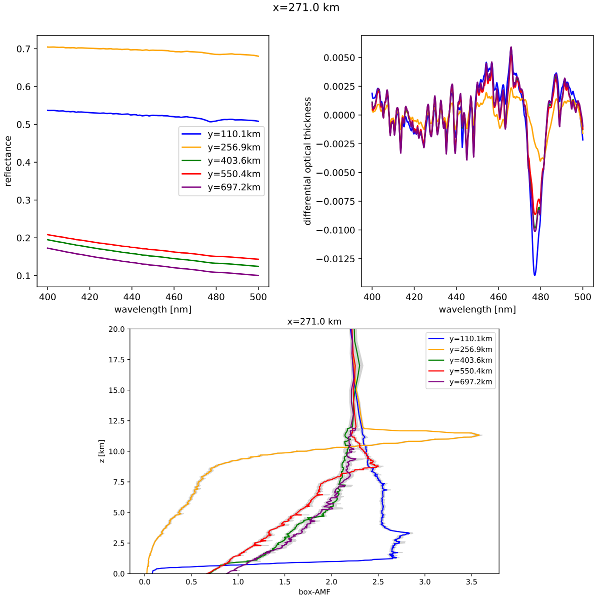
- Spectral range: 400-500 nm (0.2 nm resolution)
- Spatial resolution approx. 7 km, 98×104 pixel
- Nadir view
- Sun position SZA: 30°, SAA: 13°
- Surface albedo: 0.05
- Molecular optical thickness profiles provided by BIRA
- NO_2-profile: European polluted
- Layer-AMF calculated at 460 nm
- ICON clouds (3D liquid and ice water content fields, spatial resolution approx. 1.2 km)

Reflectance simulation

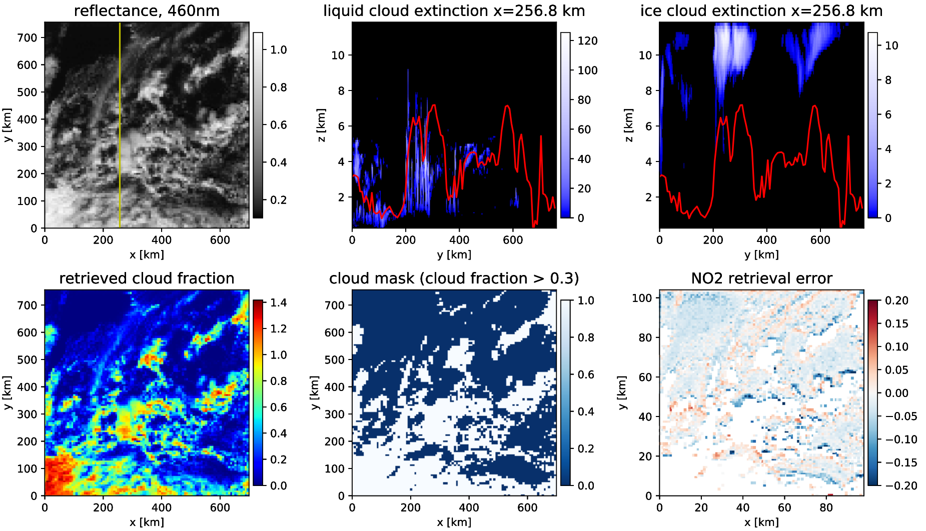




Reflectance spectra, DOD, and layer-AMF

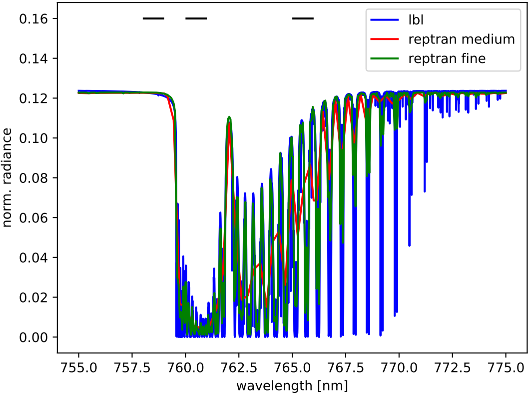


BIRA-NO2 retrieval (O_2-O_2)



Largest retrieval errors in cloud shadows

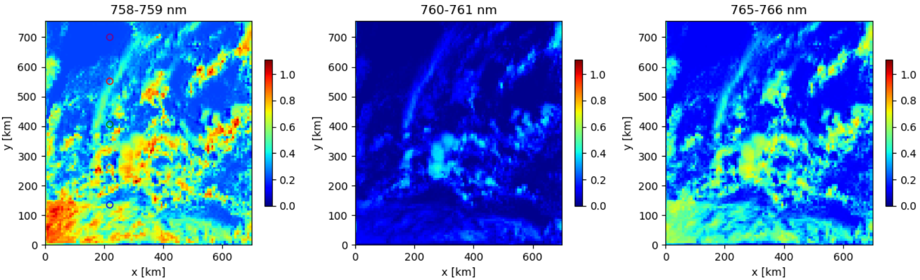
O_2A band simulations

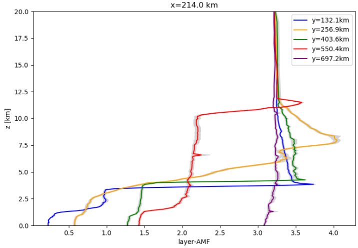


- Line-by-line (ARTS, Eriksson et al. 2011)
- REPTRAN absorption parameterization (Gasteiger et al., 2014)
- FRESCO cloud algorithm uses averages over bands 758–759 nm, 760–761 nm, 765–766 nm.

REPTRAN (fine spectral resolution) accuracy sufficient to calculate band averages, saves storage memory and CPU time

Reflectance and layer-AMF simulations in O_2A band



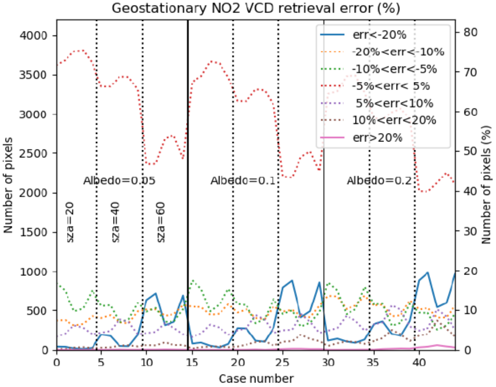


Synthetic dataset for LES cloud scene

	Geostationary Orbit	Low Earth Orbit
solar zenith angles [°]	20,40,60	20,40,60
solar azimuth angles [°]	-90, 45,0,45,90	13, 353
sensor viewing zenith angle [°]	58.3	0,20,60
sensor viewing azimuth angle [°]	196.3	109.5, 281.7
surface albedo	0,0.05,0.2, (0.5 for O_2A band)	

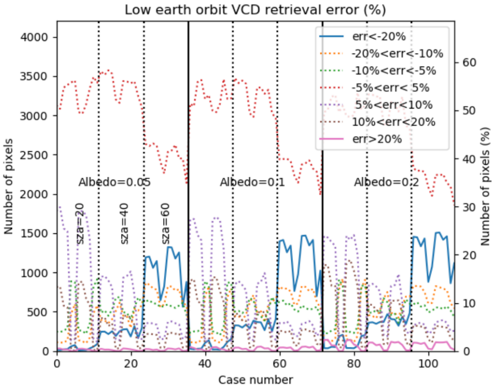
Table: Representative sun positions, sensor viewing directions and surface albedos included in synthetic dataset. 45 combinations for GEO and 108 for LEO.

NO_2 retrieval error statistics - GEO



- average medium bias: -0.9%
- between 61% (high albedo) and 93% (low albedo) of the retrieved NO_2 VCD are within 10% of the “true” column
- number of pixels with differences $<$-20% increase from about 0.2% for low albedo and high sun to up to 22% for high albedo and low sun
- The variation within each SZA interval is due to different SAA

NO_2 retrieval error statistics - LEO



- average median bias: -0.5%
- between 53% (high albedo) and 89% (low albedo) of the retrieved NO2 VCD are within 10% of the actual column
- number of pixels with differences $<$-20% increase from about 0.1% for low albedo and high sun to up to 26% for high albedo and low sun
- Within each SZA interval the SAA angle takes two values, results are similar for these two angles
- largest differences within each SZA interval are found when VZA is large (60°)

Summary

- One-dimensional simulations
  - Ensure that MYSTIC and LIDORT agree for clear-sky cases
  - Test cloud correction algorithm (O_4 and FRESCO) for 1D cloud cases
- Box cloud simulations
  - (3D) Box-airmass factor simulations
  - Simulation of reflectance spectra for clear pixels influenced by near clouds
  - Impact of solar zenith angle, albedo, cloud optical thickness, cloud geometrical thickness and cloud bottom height on NO_2 retrieval error
- Comprehensive synthetic dataset with LES cloud input for VIS and O_2A
  - Simulated scene covers all typical cloud types for central Europe
  - Sub-pixel cloud inhomogeneity included
  - Quantification of NO_2 retrieval error due to cloud scattering