Investigation of the impact of 3D cloud scattering on operational NO_2 retrieval algorithms based on synthetic data

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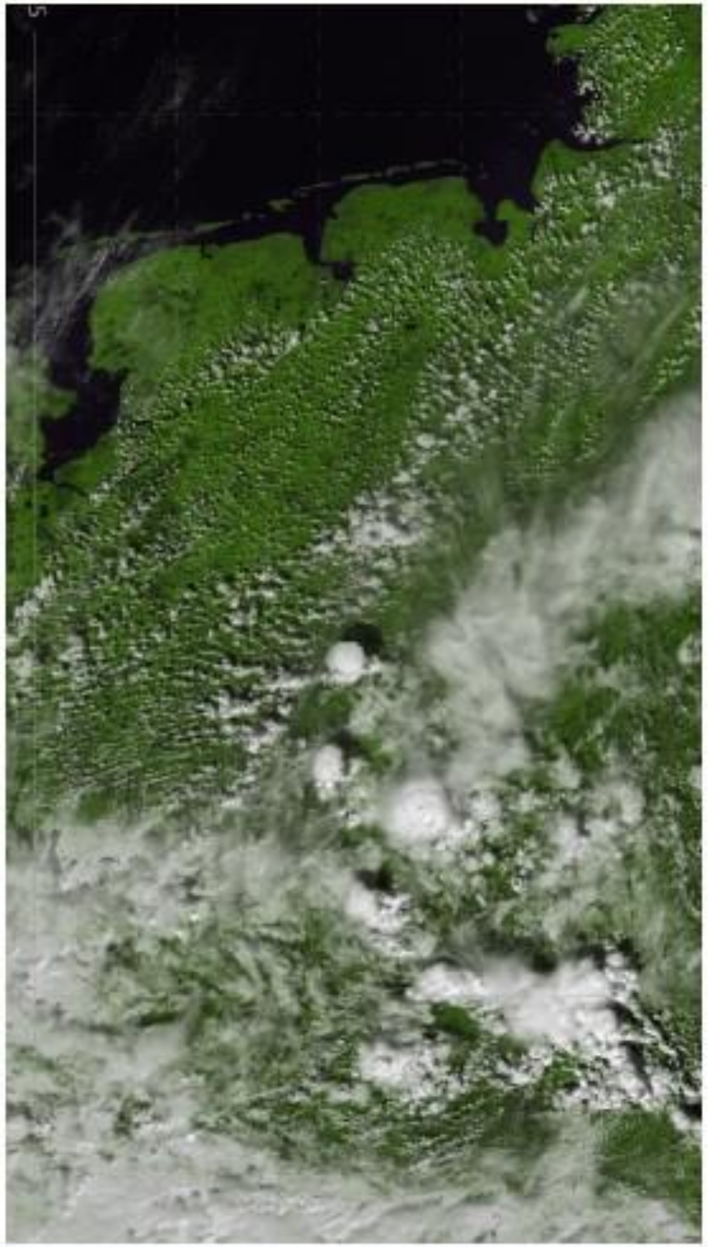
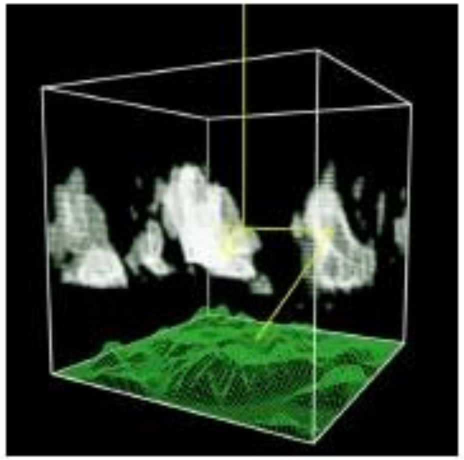
Introduction

- 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)
  ⇒ simulation of synthetic data for realistic 3D model atmospheres
- Application of NO_2 retrieval algorithms on simulated data:
- ⇒ quantification of retrieval error due to 3D cloud scattering
- ⇒ enables comparison and validation of different retrieval approaches



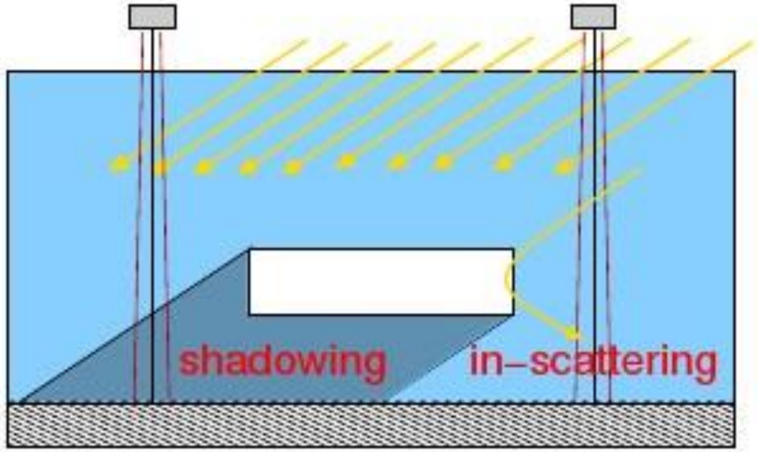
Radiative transfer model MYSTIC



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

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

Synthetic data I: Box cloud setup



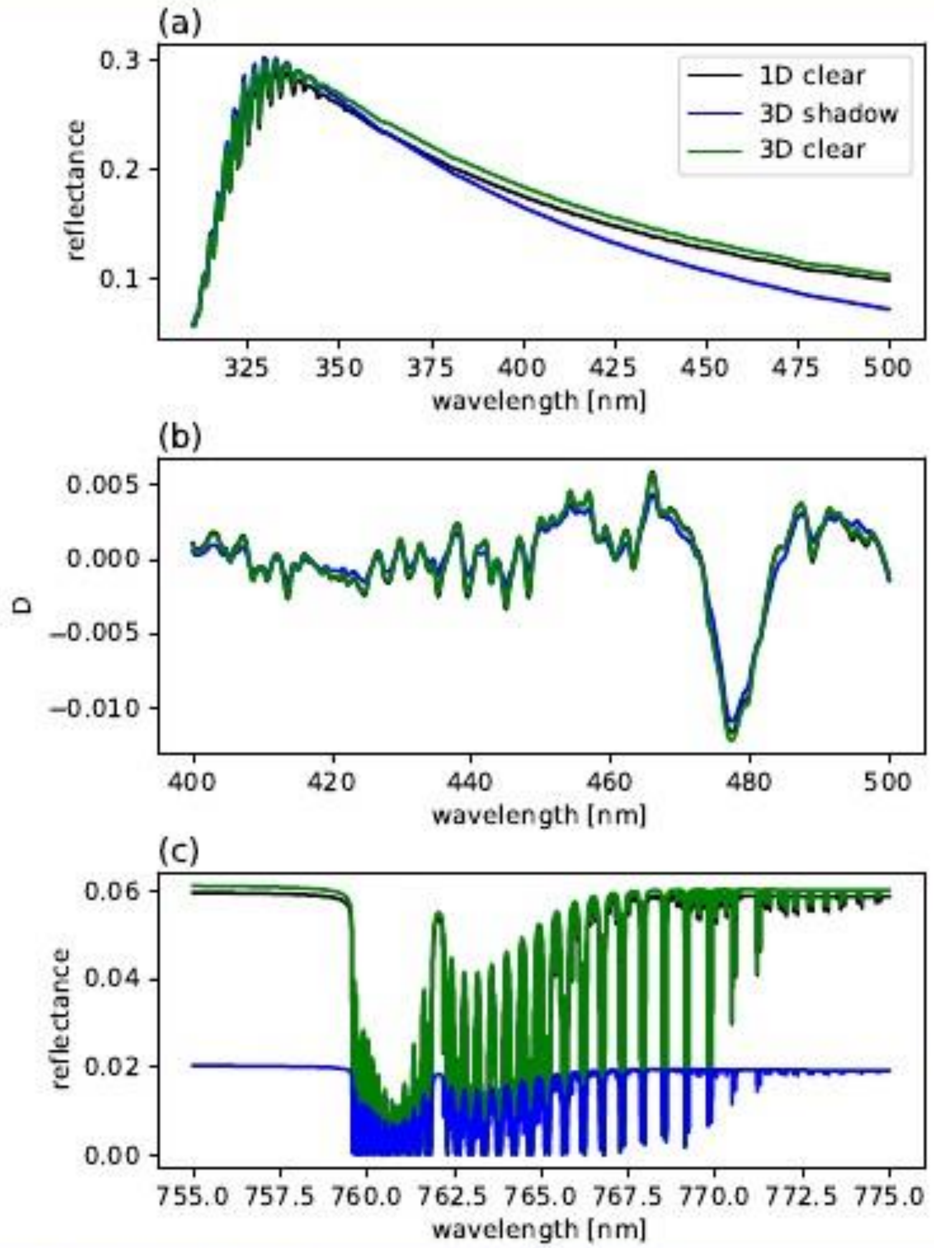
Sketch of box cloud setup.

General settings

- nadir observation geometry
- $1x1km^2$ square field-of-view
- NO_2 profiles: Pacific polluted, European polluted
- surface albedo: 0.05
- no aerosol
- spectral resolution VIS: 0.2nm, O2A: 0.005nm

	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	

Output: Synthetic data



- Spectra in UV/VIS (300-500nm) and O2A-band (755-775nm)
- Box airmass factors (450nm)

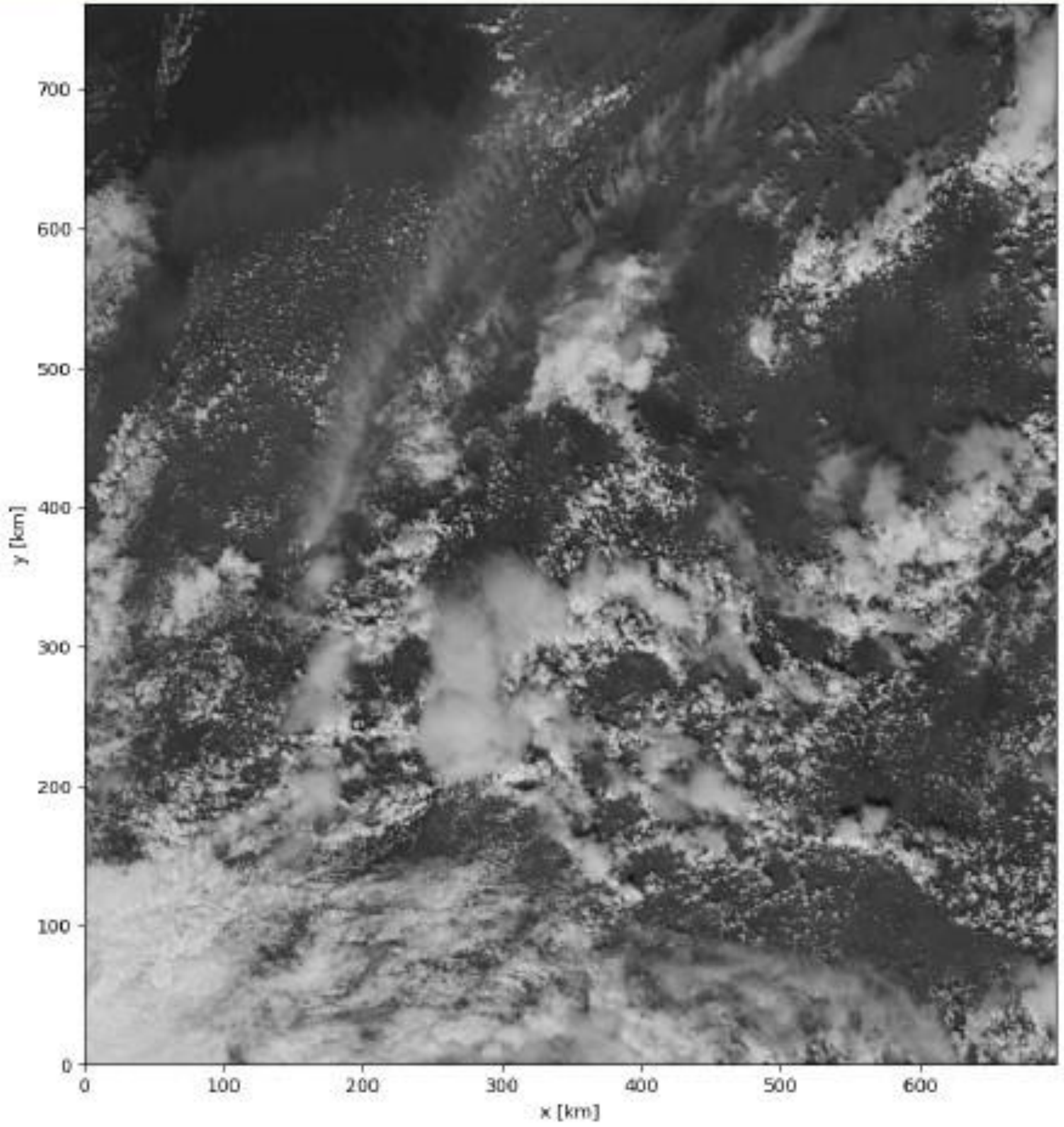
1.5 km away from cloud (shadow)

10.5 km away from cloud (clearsky)

Synthetic data II: LES cloud scenario

MYSTIC input from ICON model (Dipankar et al. 2015, Zängl et al. 2015)

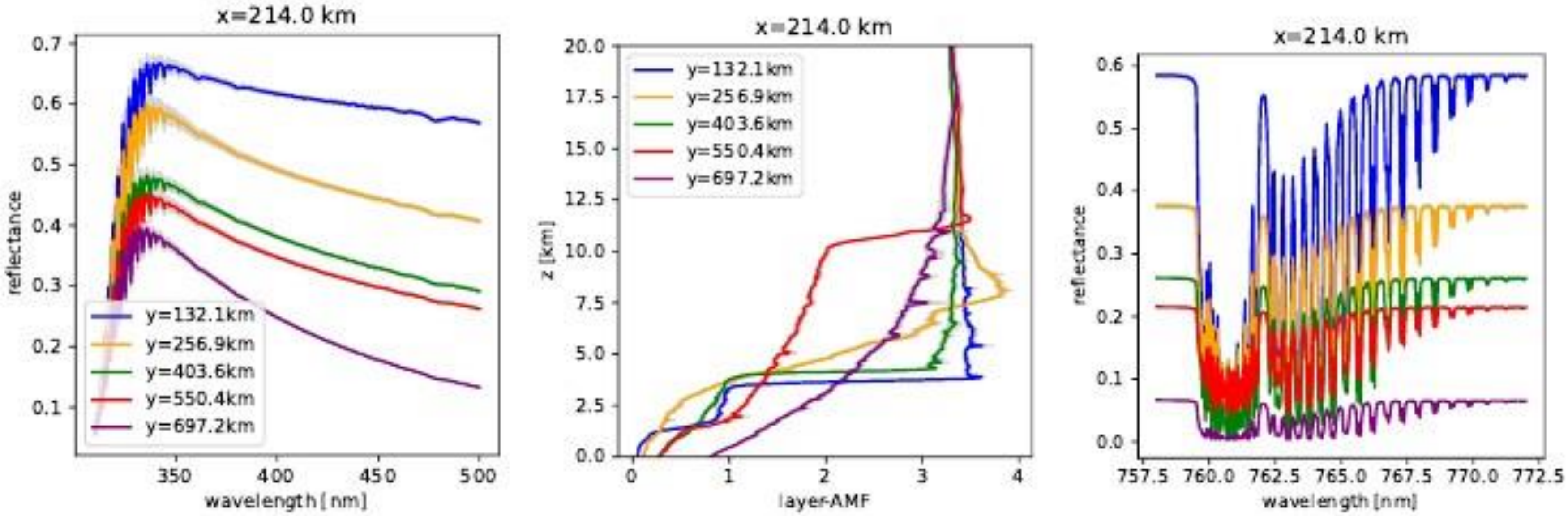
- Spatial resolution approx. 1 km for region including Germany, Netherlands and parts of other surrounding countries
- ICON validated against ground-based and satellite based observational data (Heinze et al. 2017, Emde et al. 2022)
- Simulations include all cloud types that are typical for Europe (e.g. shallow cumulus, cirrus, stratus, and convective clouds)



Simulated satellite image with MYSTIC.

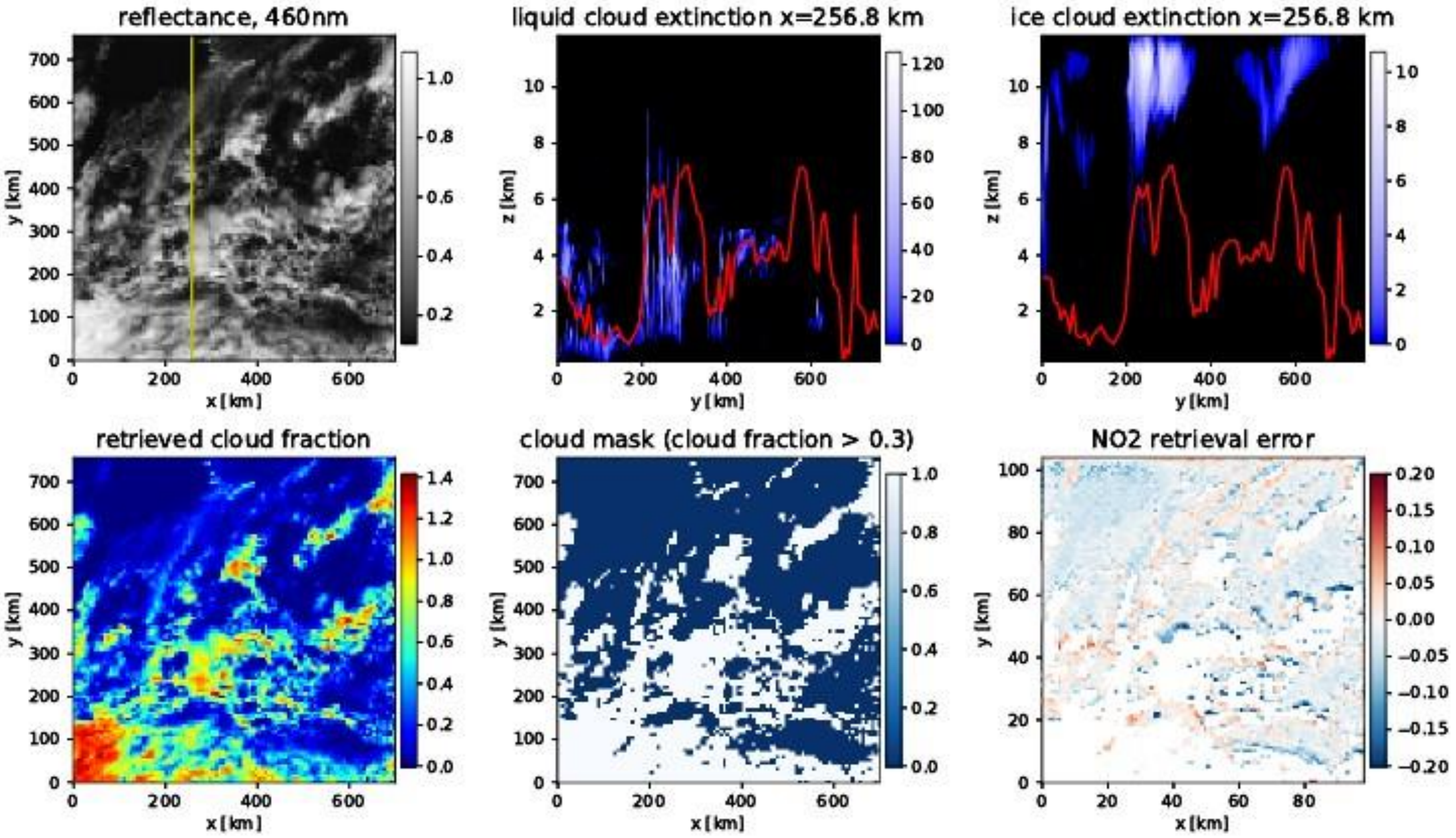
Synthetic data II: LES cloud scenario

- Representative sun positions, sensor viewing directions and surface albedos, 45 combinations for GEO and 108 for LEO
- Spectra in UV/VIS and O2A band
- Spatial resolution ≈7km, subpixel heteorogeneity, multi-layer and mixed-phase clouds included



Dataset freely available at
`https://doi.org/10.5281/zenodo.5567616.`

3DCATS: Quantification of NO_2-VCD retrieval error



BIRA-NO2 retrieval (O_2-O_2): Largest retrieval errors in cloud shadows

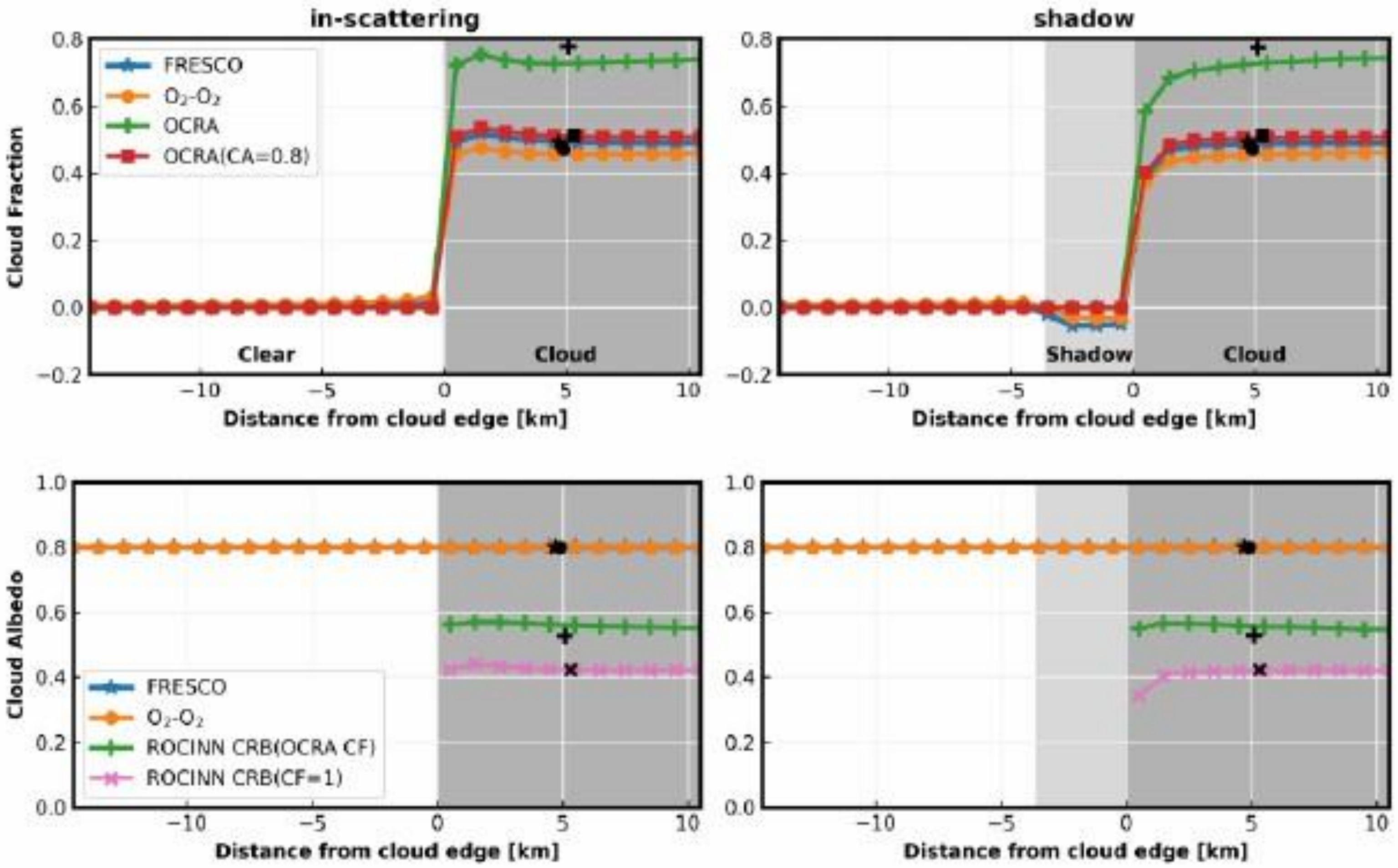
Emde et al. 2022, Yu et al. 2022, Kylling et al. 2022 (AMT)

3DCTRL: Validation of cloud correction schemes based on synthetic data

Cloud correction schemes:

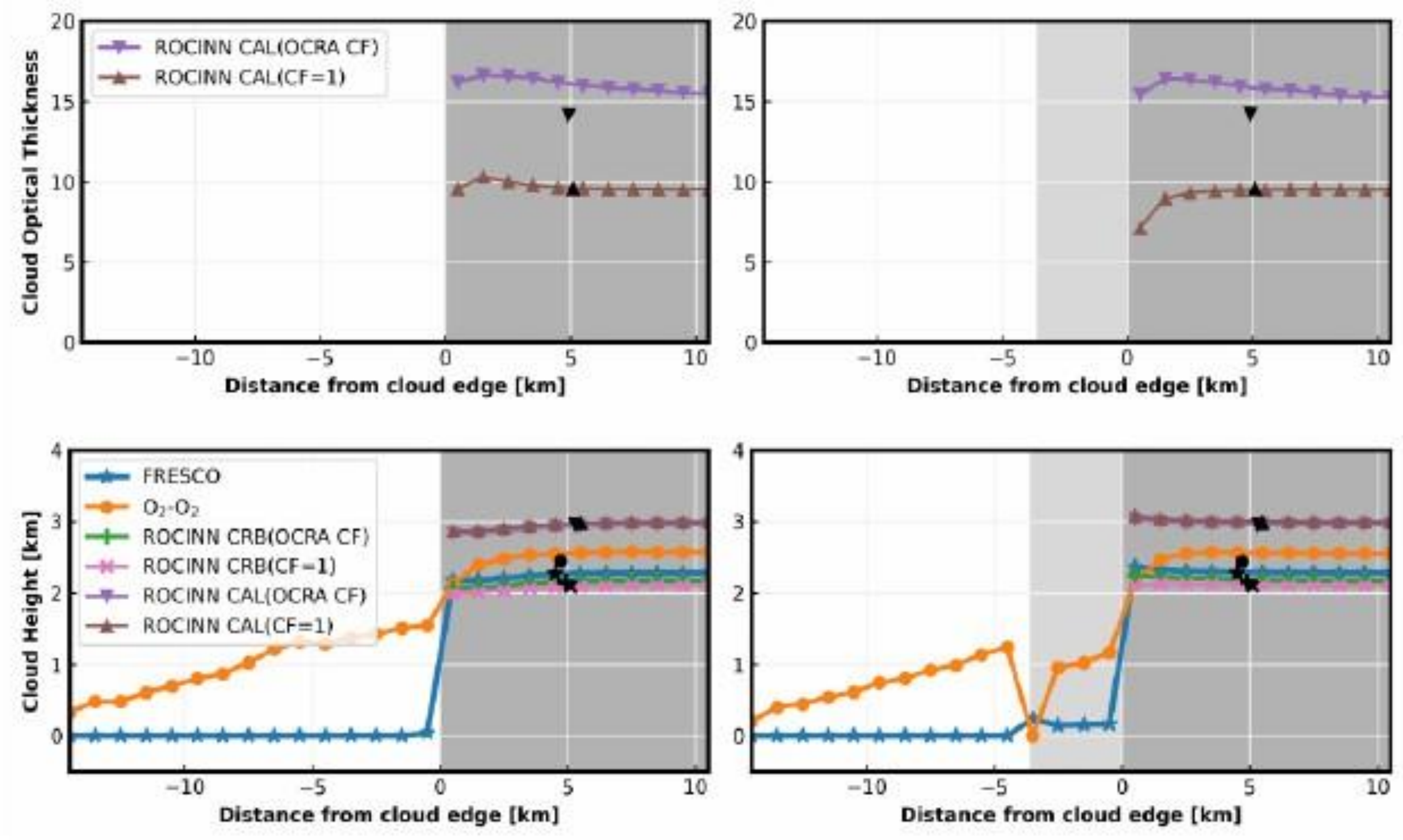
1. FRESCO (based on O_2A band)
2. O_2-O_2
3. OCRA/ROCINN CRB (cloud as reflecting boundary)
4. OCRA/ROCINN CRB with adapted scaling for cloud fraction and cloud albedo=0.8
5. OCRA/ROCINN CAL (cloud as layer)
6. ROCINN CAL with a fixed cloud fraction of 1

Cloud retrieval validation for 2D box cloud scenario



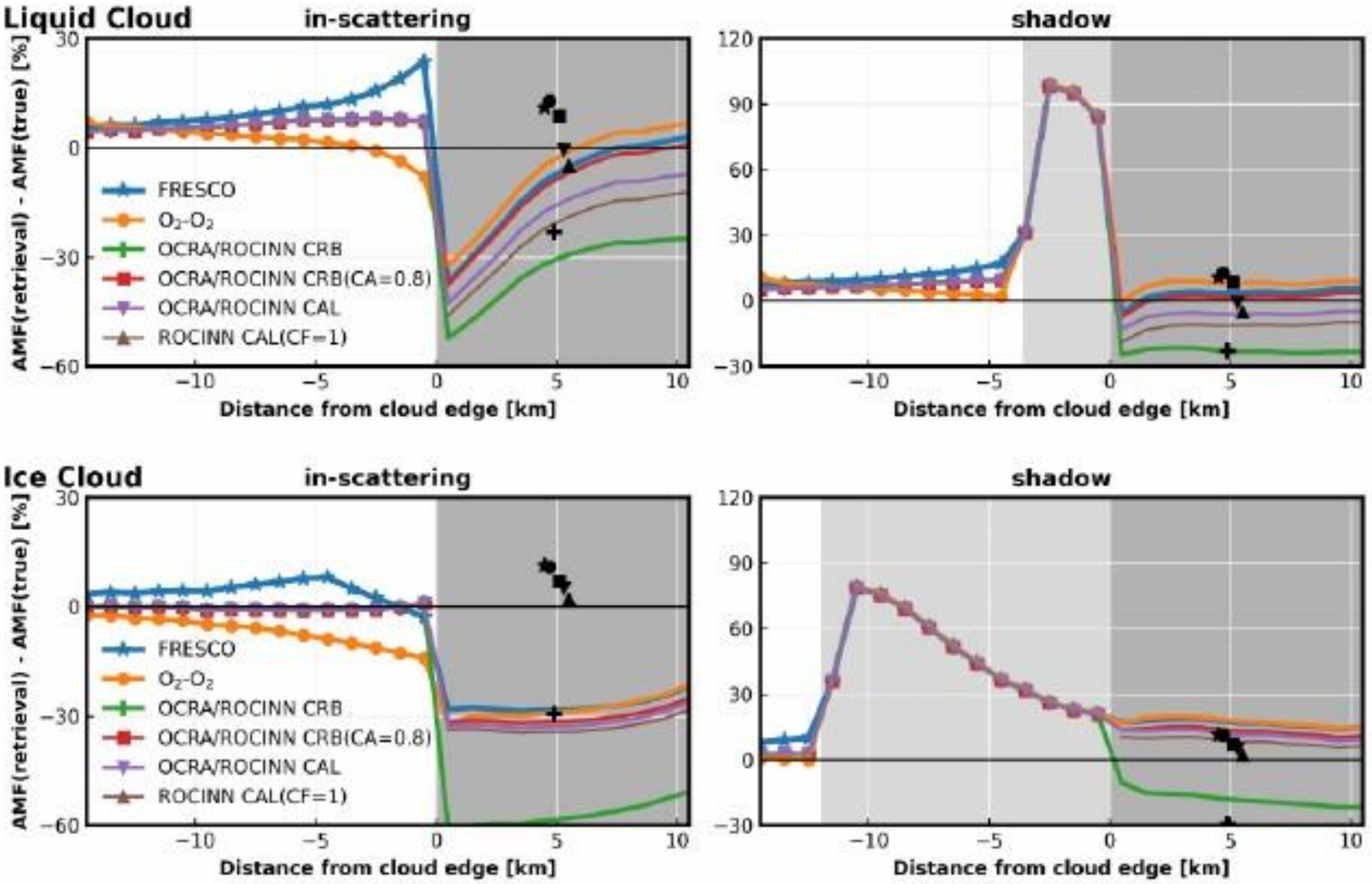
Cloud fraction and cloud albedo retrievals for liquid water cloud as a function of distance from the cloud edge (CRB models).

Cloud retrieval validation for 2D box cloud scenario



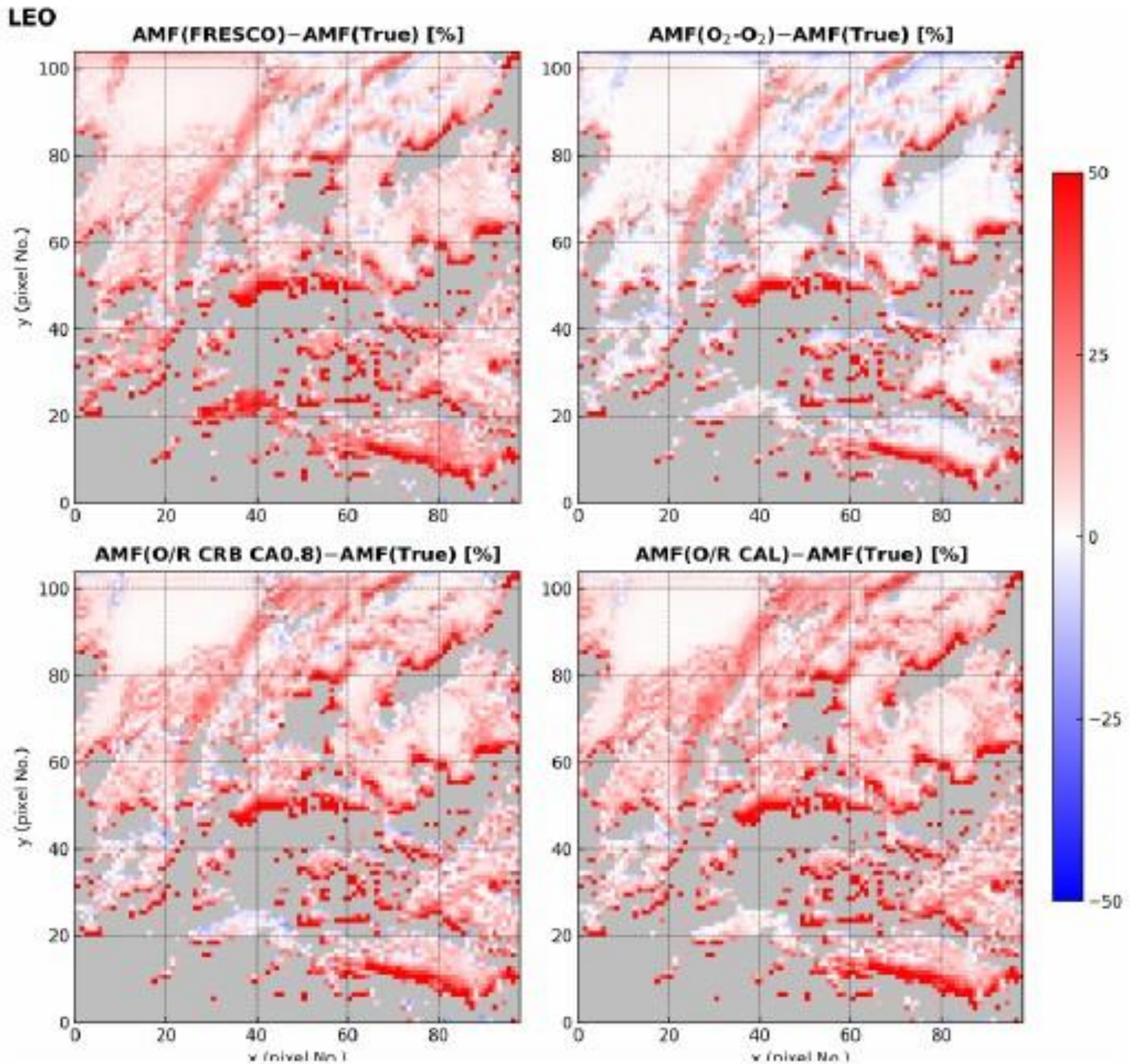
Cloud optical thickness (only CAL) and cloud height retrievals for liquid water cloud as a function of distance from the cloud edge.

AMF retrieval bias for 2D box cloud



AMF bias as a function of distance from cloud edge.

AMF retrieval bias for LES clouds



Mean bias of the AMF based on various cloud corrections for all LEO cases (50% in cloud shadows).

Similar patterns for all algorithms.

Summary of validation based on synthetic data

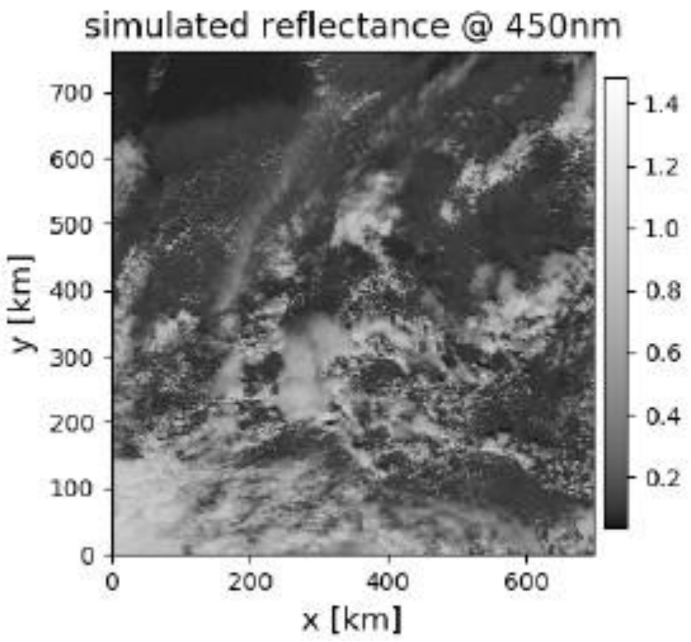
- Comparison of six NO_2 retrieval algorithms: FRESCO, O_2-O_2, OCRA/ROCCIN (CRB, CRB/0.8, CAL, CAL/1.0)

- 1D cloud layer
  - NO2-VCD retrieval bias below 20%
- 2D box cloud scenario
  - AMF overestimation in cloud shadows
  - AMF underestimation in clouds
- Realistic LES cloud scenario
  - Mostly positive AMF bias$\Rightarrow$ underestimation of NO_2-VCD
  - Largest mean bias in cloud shadows ($\approx$50%)
- Outlook
  - Cloud shadow product $\Rightarrow$ correct NO_2 retrieval bias
  - Investigate retrieval accuracy for other trace gases

Appendix

Summary of synthetic dataset

- Cloud setups with different complexities
  - (a) 1D cloud
  - (b) 2D box cloud
  - (c) broken clouds from LES simulation
- Typical sun-observer geometries for LEO and GEO orbits
- Extended 3DCATS dataset to OCRA/ROCCIN requirements
  - Sentinel-S5P band 3 (310-405nm)
  - O2A-band (758-772nm)



- Complete dataset including documentation available in 3DCTRL datapool
- Data and quicklooks also available at `https://www.meteo.physik.uni-muenchen.de/~emde/doku.php?id=projects:3dctrl:3dctrl_synthetic_dataset`

libRadtran

http://www.libradtran.org
1991 – 2022
Mayer und Kylling, ACP, 2005.
Emde et. al, GMD, 2016

spectral range	UV, visible, infrared (250nm-100μm)
model geometry	plane-parallel, spherical, three-dimensional
observer position	surface, air-borne, satellite
absorption	quasi-spectral, correlated-k, line-by-line
RT solvers	DISORT, Monte Carlo, twostream, ...
output quantities	(polarized) radiance, irradiance, heating rate, actinic flux

- Optical properties parameterizations for clouds and aerosols
- Mie tool
- Single scattering lidar and radar simulators

- Validated in various model intercomparison studies
- More than 1000 peer-reviewed publications that used libRadtran
- Development partly funded by ESA (ESASLight I+II)

3D radiative transfer in high spectral resolution

NO_2 retrieval (DOAS) – fit differential optical thickness

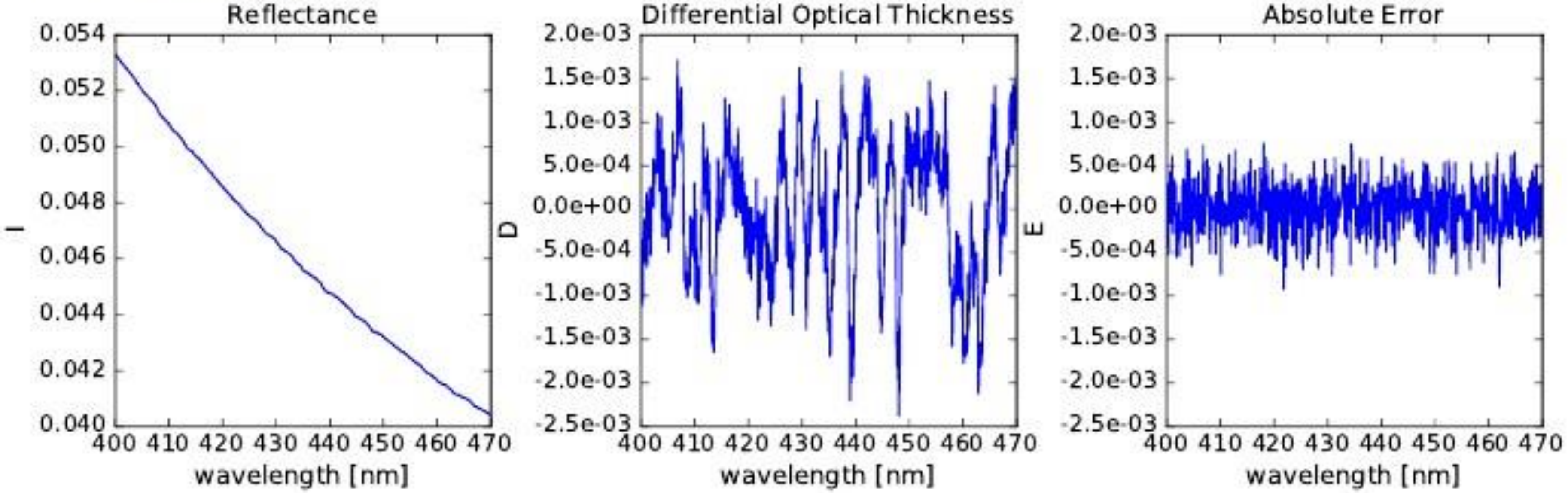
$$D(\lambda) = \ln(I_{TOA}(\lambda)) - P_3(\lambda)$$

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!)

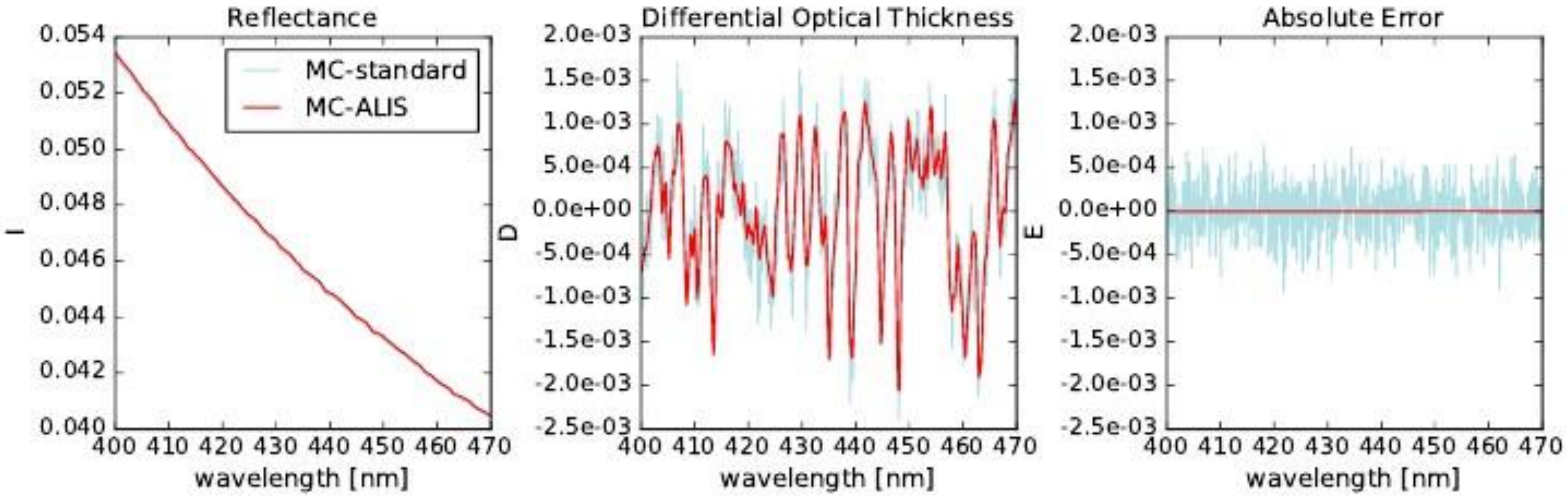
Absorption Lines Importance Sampling

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

Spectral absorption and scattering included by photon weights

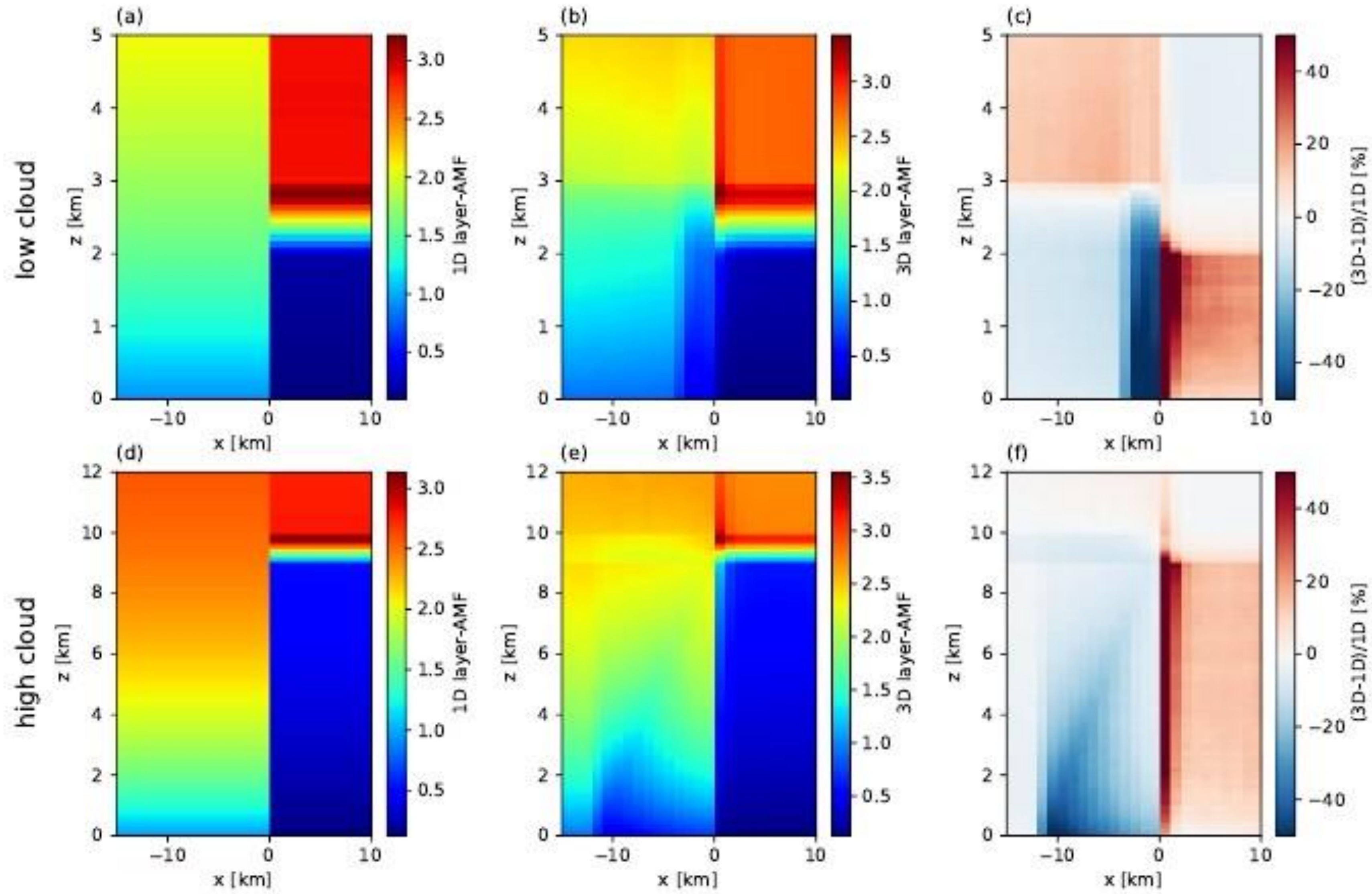
Statistical error causes bias (decreasing with $\sqrt{N}$) over full spectral range, not for each wavelength

Computational time: 1.5 minutes (comparable to DISORT)

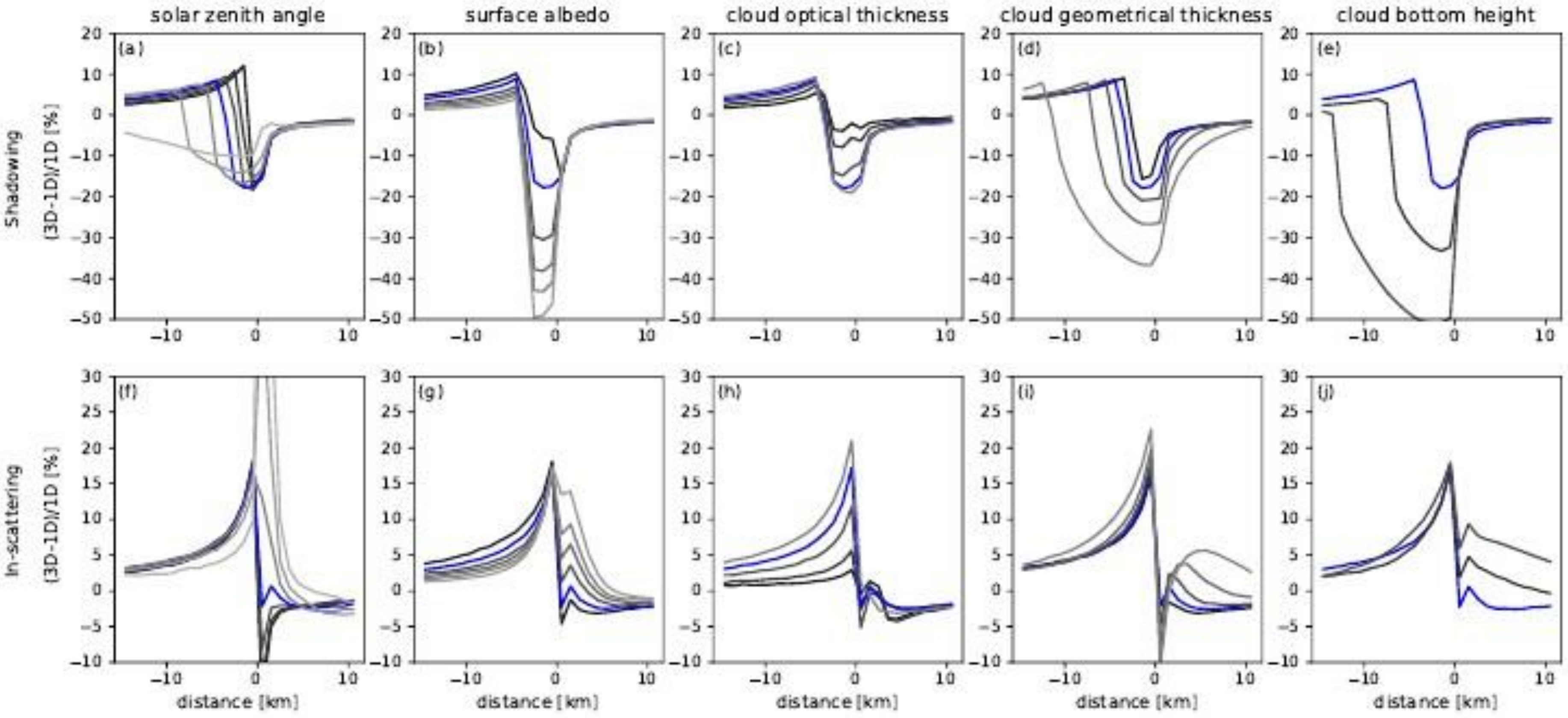


C. Emde, R. Buras, and B. Mayer. *ALIS: An efficient method to compute high spectral resolution polarized solar radiances using the Monte Carlo approach.* JQSRT, 2011

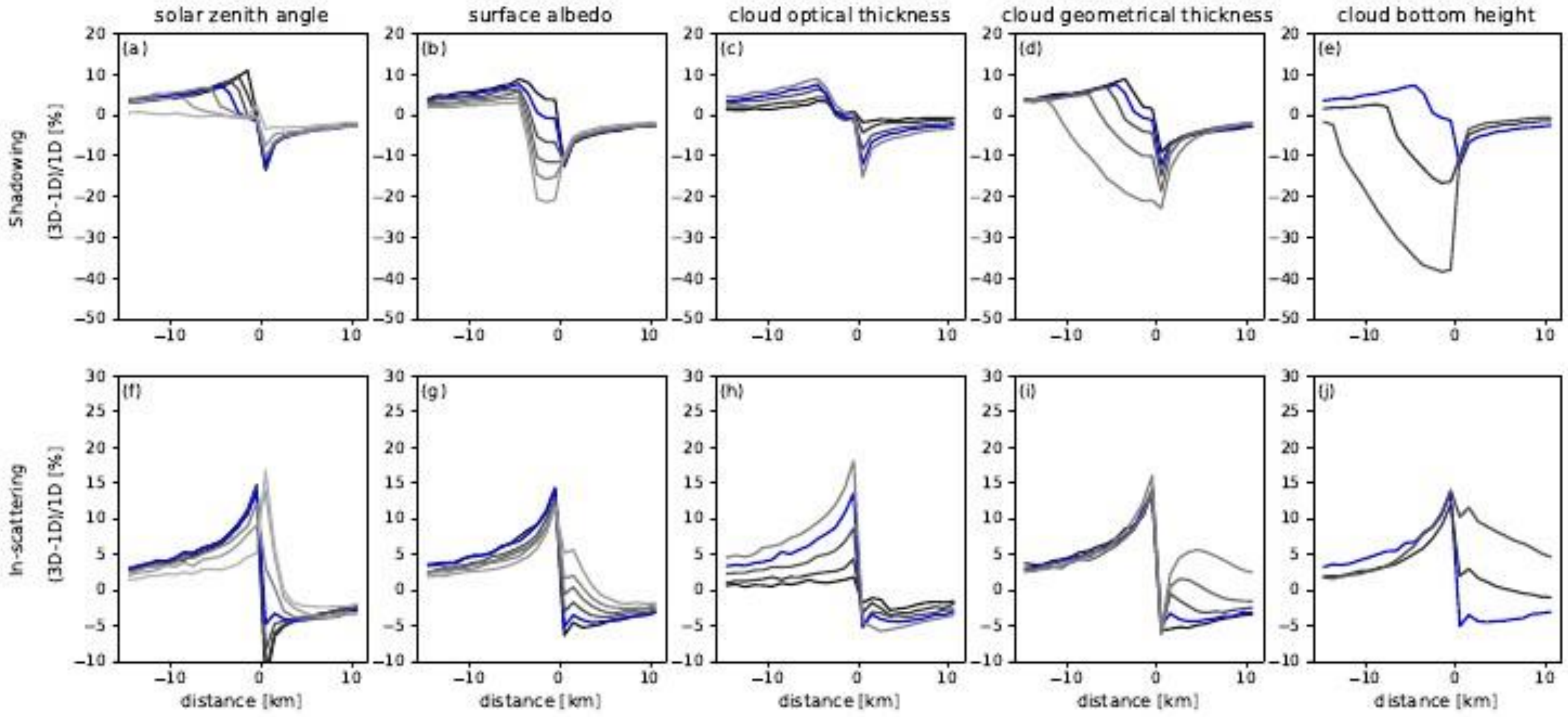
Layer airmass factors for low and high cloud (base cases)



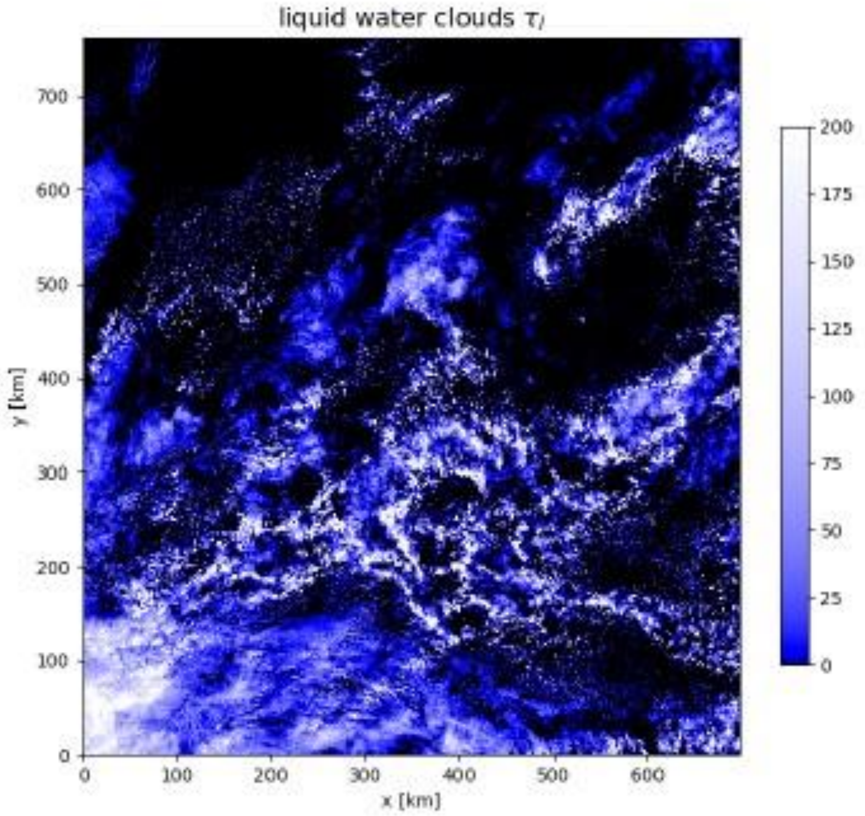
Sensitivity on various parameters @ 460nm

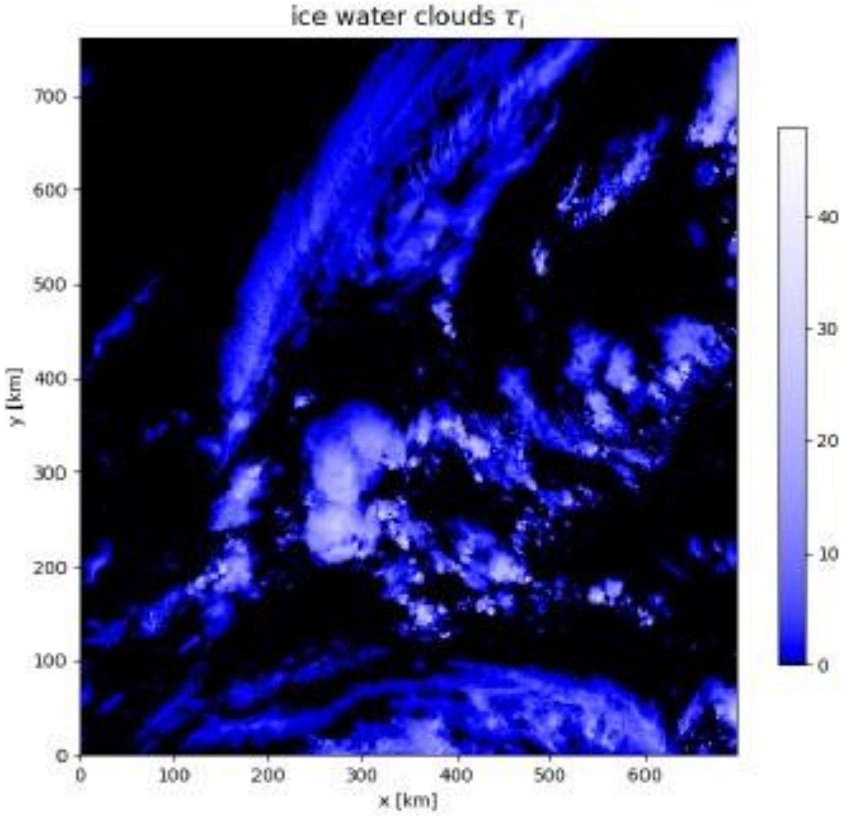


Sensitivity on various parameters @ 370nm

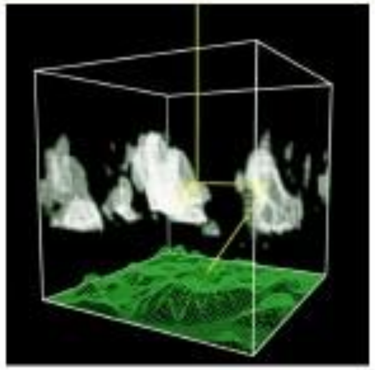


Vertically integrated cloud optical thickness





Reflectance simulation with LES clouds

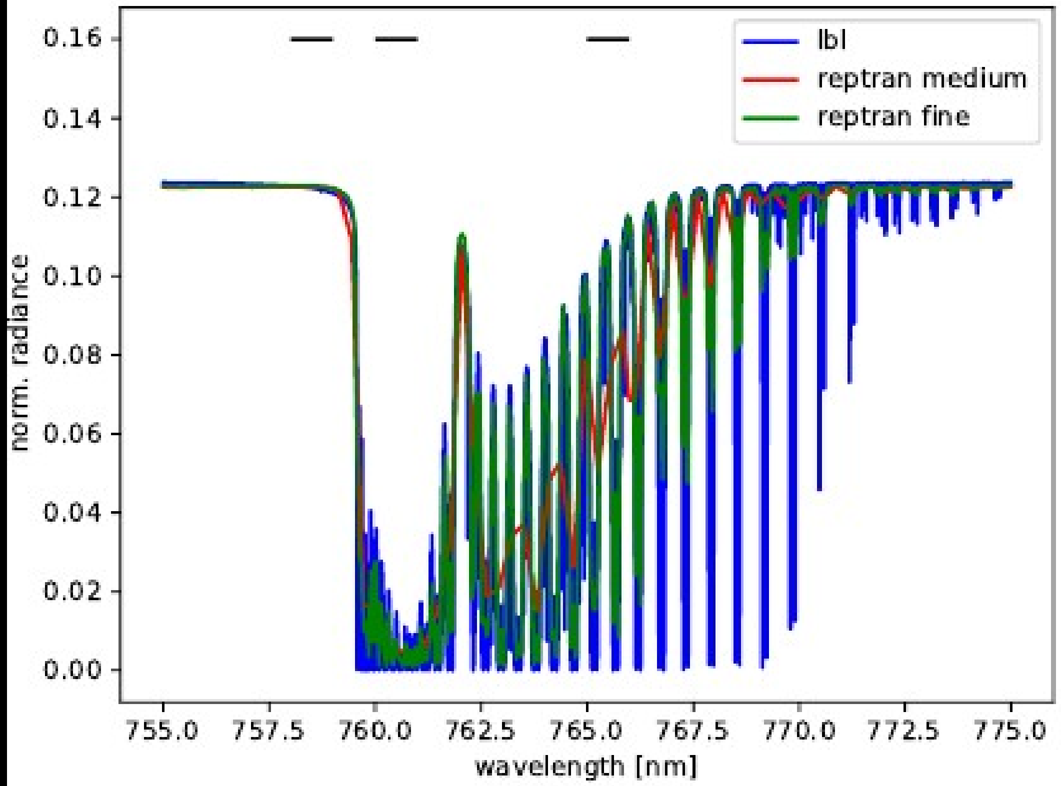


MYSTIC – Monte Carlo radiative transfer model
Mayer 2009, Emde et al. 2011, Emde et al. 2016

- 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.

O_2A band simulations



- Line-by-line (ARTS, Eriksson et al. 2011)
- REPTRAN absorption parameterization, fine resolution 0.06nm in O2A region (Gasteiger et al., 2014)
- FRESCO cloud algorithm uses averages over bands 758–759 nm, 760–761 nm, 765–766 nm.

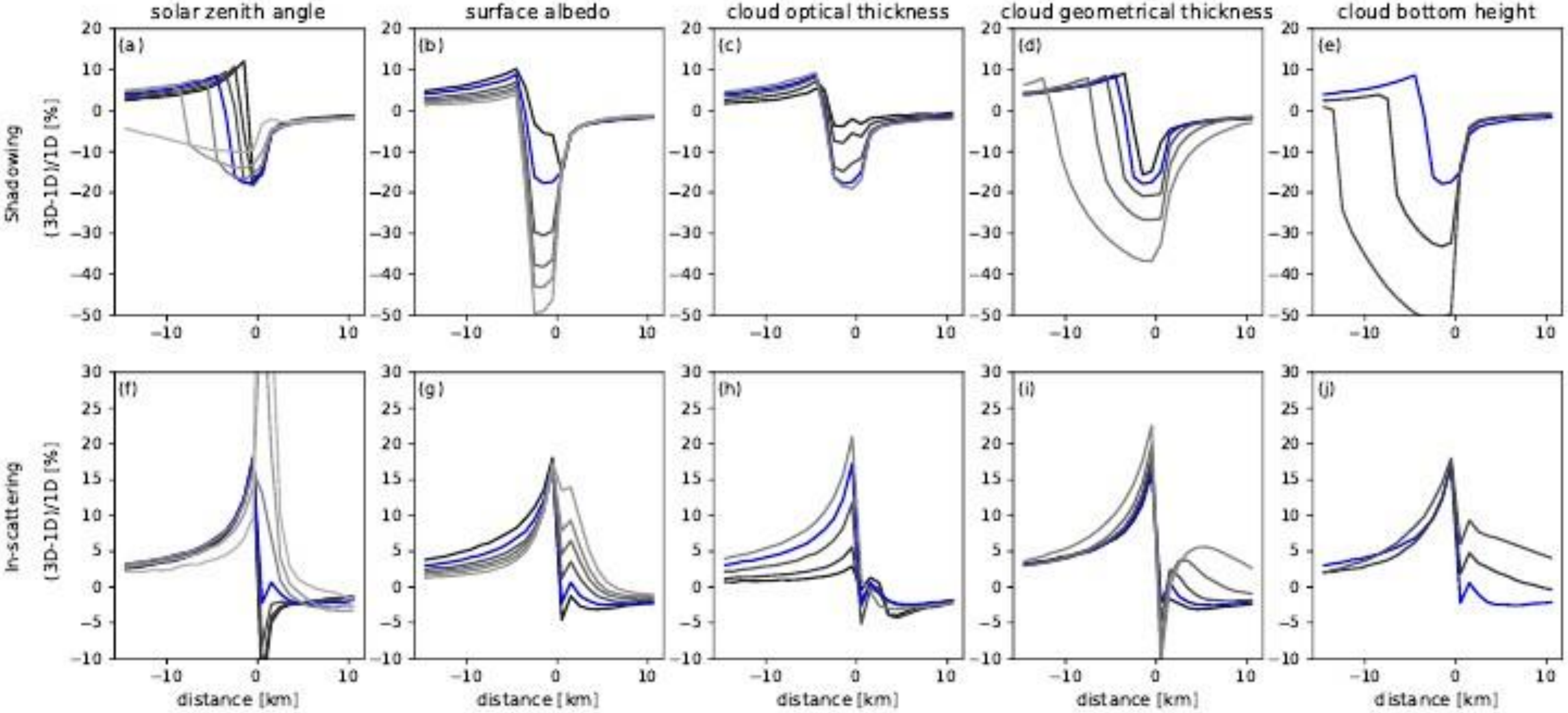
REPTRAN (fine spectral resolution) accuracy sufficient to calculate band averages, saves storage memory and CPU time

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

Sensitivity on various parameters @ 460nm

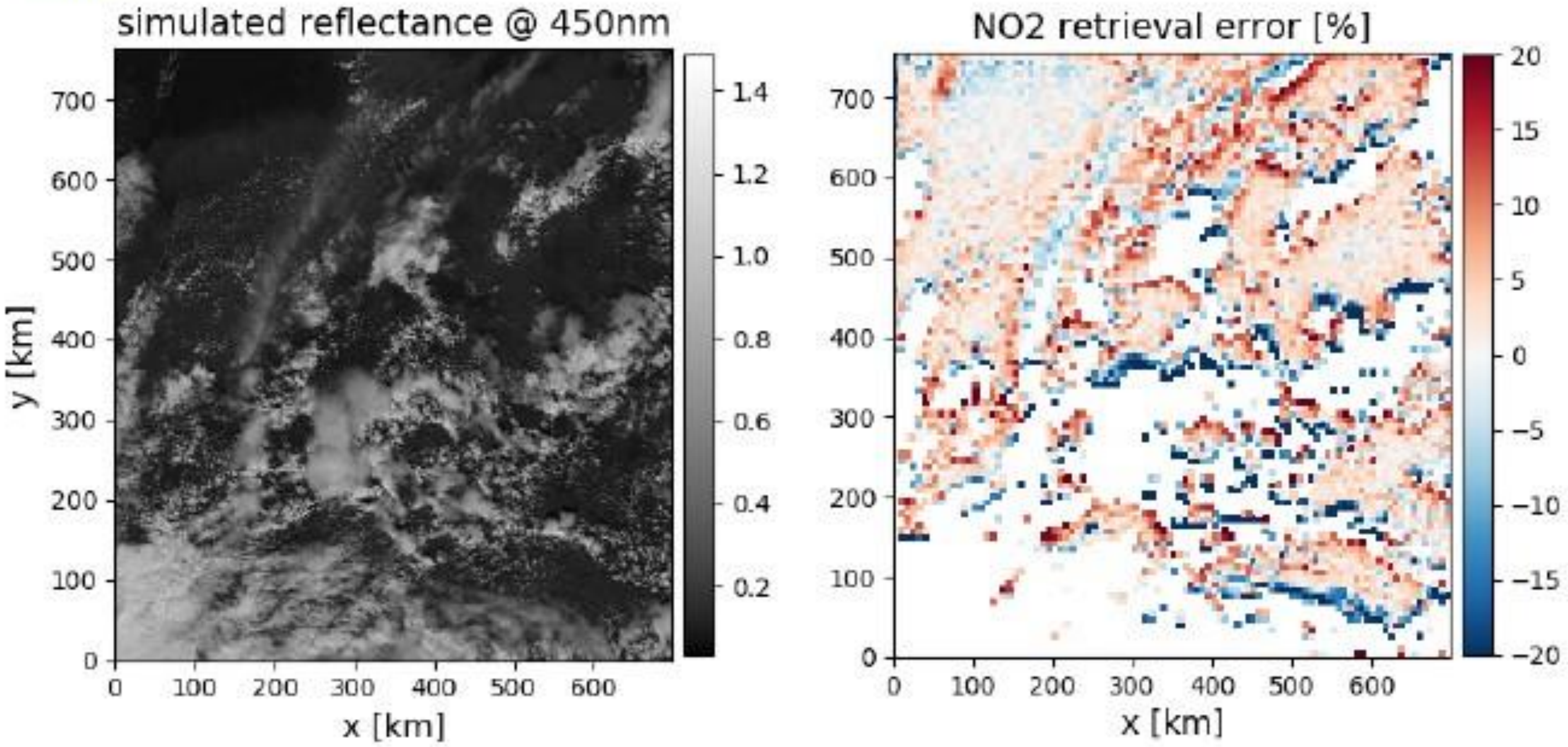


Relative difference between 3D and 1D simulations as a function of distance from cloud edge.

Quantification of NO_2-VCD retrieval error

ESA-3DCATS project:

- Emde et al., AMT 2022: Part I: Synthetic dataset for validation of trace gas retrieval algorithms
- Yu el al., AMT 2022: Part II: impact on NO2 retrieval and mitigation strategies
- Kylling et al., AMT 2022: Part III: bias estimate using synthetic and observational data



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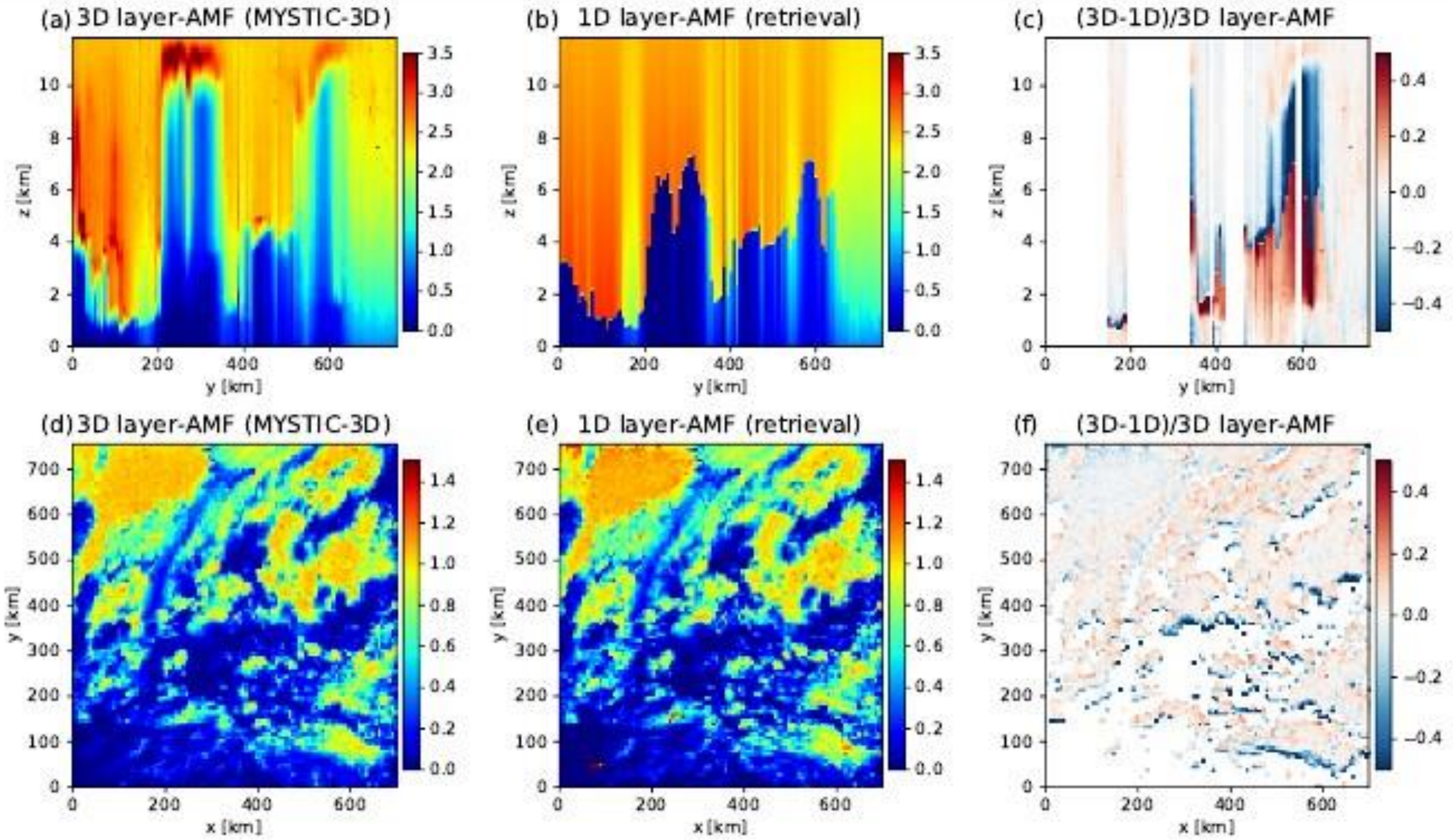

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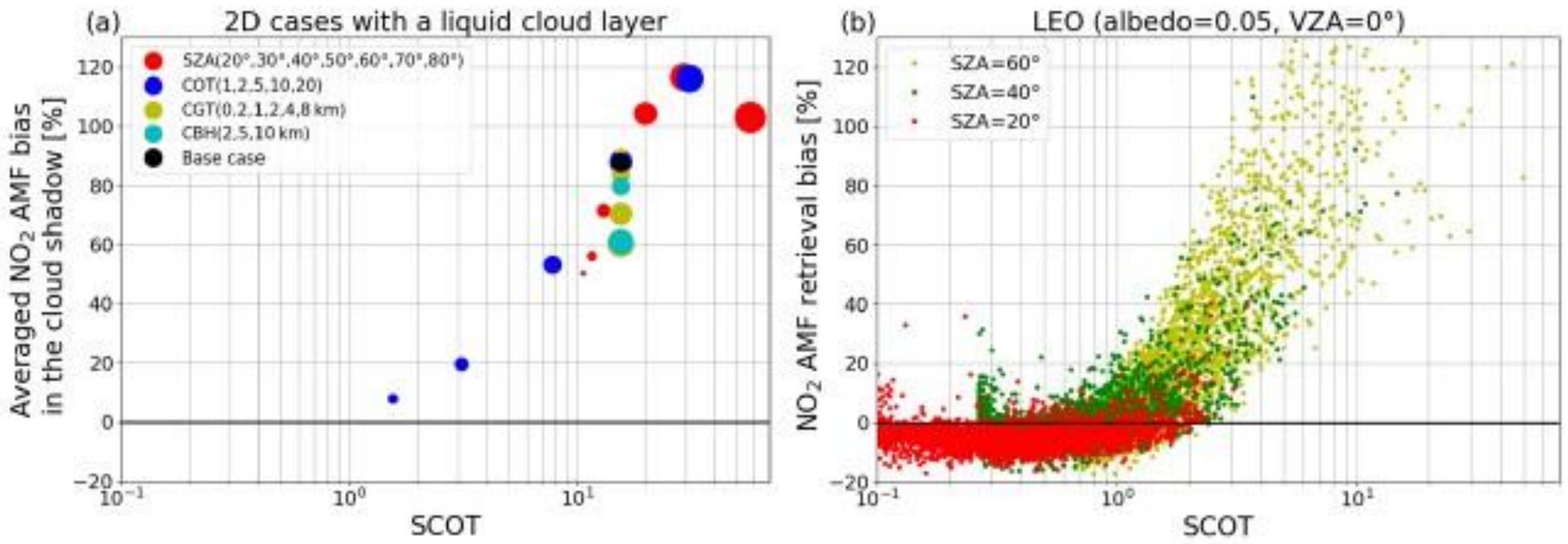
Quantification of NO_2-VCD retrieval error

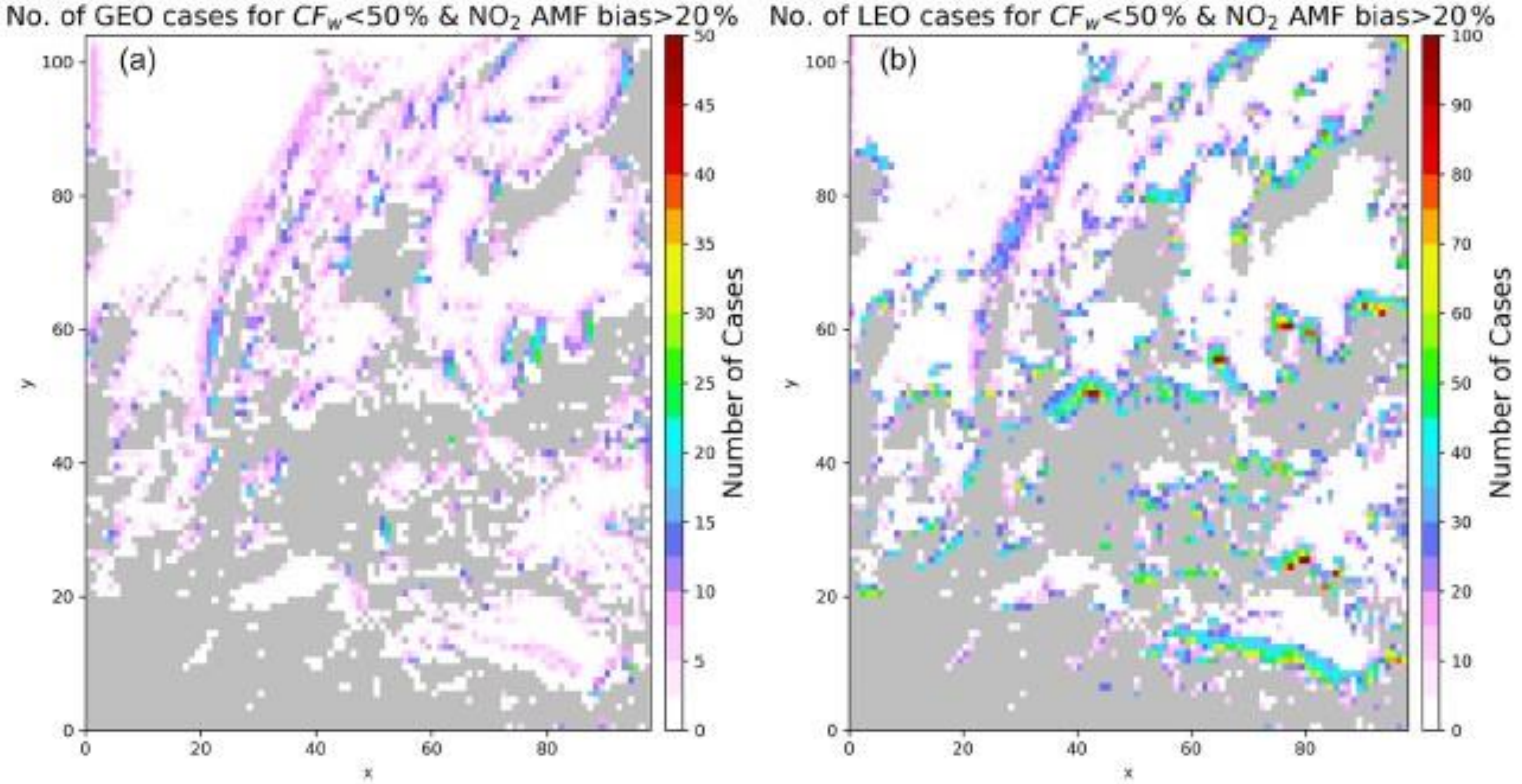


NO_2 AMF retrieval bias in cloud shadow as function of cloud optical thickness.

ESA-3DCATS Project:

Yu el al., AMT 2022: Part II: impact on NO2 retrieval and mitigation strategies

Number of cases with AMF bias >50%



Number of cases with CF<50% with AMF bias >50% for LEO and GEO.

ESA-3DCATS Project:

Kylling et al., AMT 2022: Part III: bias estimate using synthetic and observational data