Towards shortwave reflectance data assimilation for aerosols: a radiative transfer model benchmark and the 1D-Var assimilation efforts in CAMS 43

Jerónimo Escribano [1], Olivier Boucher [2], Robin J. Hogan [3], Alessio Bozzo [4],Philippe Dubuisson [5], Johannes Flemming [3], Laurent Labonnote [5], Samuel Rémy [6], Enza Di Tomaso [1] and Carlos Pérez García-Pando[1]

[1]Barcelona Supercomputing Center, Barcelona, Spain

[2]Institut Pierre-Simon Laplace, CNRS / Sorbonne Université, Paris, France

[3]European Centre for Medium Range Weather Forecasts, Reading, United Kingdom

[4]European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), Darmstadt, Germany

[5]Laboratoire d'Optique Atmospherique, Université de Lille / CNRS, Villeneuve d'Ascq, France

[6]HYGEOS, Lille, France

Outlook

Part 1:

Benchmark of short-wave radiative transfer models

Part 2:

Toy 1D-Var reflectance assimilation with synthetic observations

A benchmark for testing the accuracy and computational cost of shortwave top-of-atmosphere reflectance calculations in clear-sky aerosol-laden atmospheres

Jerónimo Escribano [1], Alessio Bozzo [2], Philippe Dubuisson [3], Johannes Flemming [4], Robin J. Hogan [4], Laurent Labonnote [3] and Olivier Boucher [5]

[1]Barcelona Supercomputing Center, Barcelona, Spain
[2]European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), Darmstadt, Germany
[3]European Centre for Medium Range Weather Forecasts, Reading, United Kingdom
[4]Laboratoire d'Optique Atmospherique, Université de Lille / CNRS, Villeneuve d'Ascq, France
[5]Institut Pierre-Simon Laplace, CNRS / Sorbonne Université, Paris, France

2 x AC science talks: Radiance assimilation for aerosols, ECMWF, 23/01/2020

Need of a SW benchmark

CAMS43 - WP3 aim : data assimilation of reflectance for aerosols

- Choose a model to perform 1D-Var reflectance assimilation in research mode
- Have to be **accurate** enough
- Have to be **fast** enough
- Performant under realistic aerosol-laden conditions

Requirements of RTM

- Short-wave
- Accuracy : close to model and observation accuracy
- Computing time : no larger than 10 times RTTOV infrared calculations (ie, about 1 ms per profile) in ECMWF/CAMS infrastructure
- Tangent linear and adjoint

Need of a SW benchmark

Benchmark design limitations

- Clear-sky
- Limited set of chosen surface and geometry
- Only direct mode (no adjoint, no tangent linear)
- No mixtures of aerosols
- One atmospheric vertical profile
- One aerosol vertical profile
- Plane-parallel
- Choice of reference model

Input data and definitions

Test with 4 models

Benchmark: 44080 cases

Wavelengths
470, 550, 660, 865, 1024 nm

Geometry
- Solar zenith angles :
  0, 20, 40 and 60 degrees
- Viewing zenith angles :
  0, 20, 40 and 60 degrees
- Azimuthal angles :
  0, 45, 90, 135, 180 degrees

Midlatitude summer atmospheric profile (49 layers)
- Molecular absorption and scattering optical depth
- Pressure, temperature, . . .

Aerosol types Industrial scattering, Industrial absorbing, Dust, Sea salt
- Phase function (S_{11}, S_{12}, S_{33}, S_{34})
- Generalized spherical decomposition (Legendre moments)
- Single scattering albedo
- Extinction efficiency, size distribution parameters, refractive indexes ...

Aerosol optical depth (AOD,550 nm)
0,0.01, 0.05, 0.1, 0.2, 0.5, 1, 2
Aerosol profile exponential with 2 km height scale

Surface reflectance
- Lambertian reflectance : 0, 0.05, 0.1
- Cox-Munk BRDF (Mishchenko and Travis, 1997)

Models

DISORT (version 4)

- Discrete ordinary method
- Scalar
- Stamnes et al. (1988)
- 32 streams, TMS correction

6SV2 (version 2.1)

- Successive orders of scattering
- Vector
- Vermote et al. (1997); Kotchenova and Vermote (2007)
- Three elements approximation (I, Q, U)

VLIDORT (version 2.7)

- Discrete ordinary method
- *Scalar* and Vector
- Spurr (2008, 2014)
- 32 streams, TMS correction
- Output jacobians

FLOTSAM

- Forward-Lobe Two-Stream Radiance Model
- Two-stream + phase function decomposition
- Scalar
- Developed by Robin Hogan
- Output tangent linear and adjoint

Reference : VLIDORT - vector

Outputs and metrics

Reflectance

$$\rho_l = \frac{\pi \ l}{l_s \ \cos(\theta_s)}$$

CPU time (single-thread, exclude I/O)

- One call - one output
- One call - multiple output

Metrics

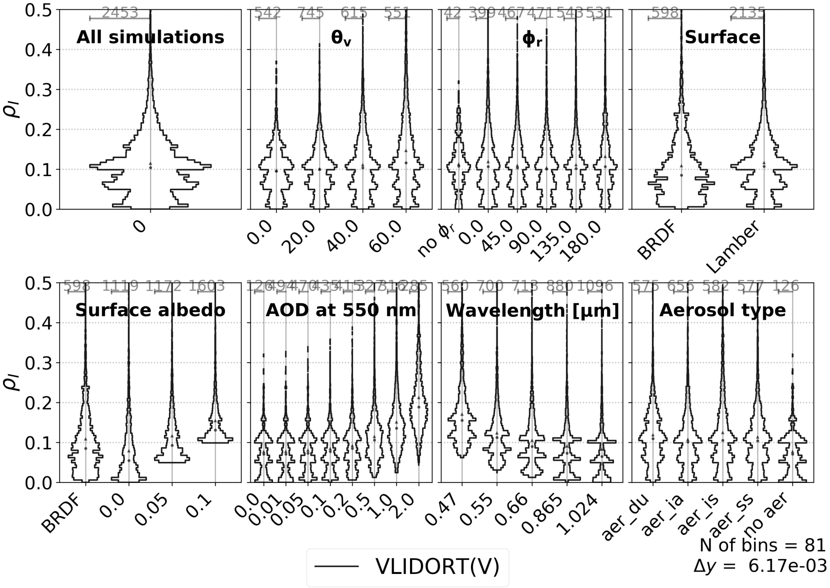
$$\text{Root Mean Square Error (RMSE)} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(m_i - r_i)^2}$$

$$\text{Mean Fractional Bias (MFB)} = \frac{2}{N}\sum_{i=1}^{N}\frac{m_i - r_i}{m_i + r_i}$$

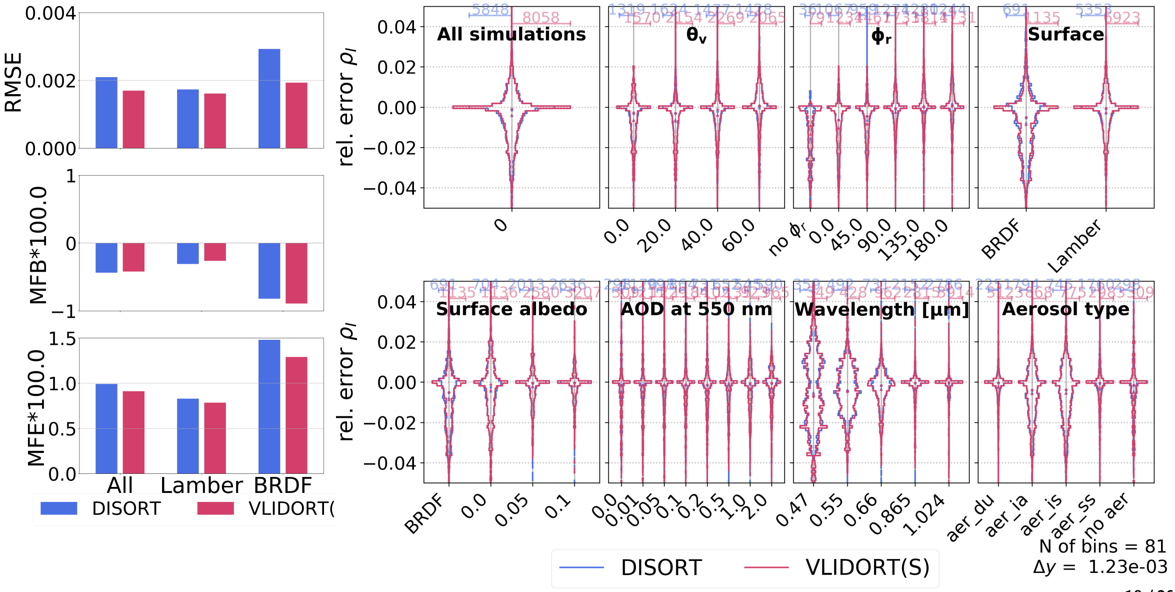
$$\text{Mean Fractional Error (MFE)} = \frac{2}{N}\sum_{i=1}^{N}\left|\frac{m_i - r_i}{m_i + r_i}\right|$$

m_i : model ; r_i : model reference

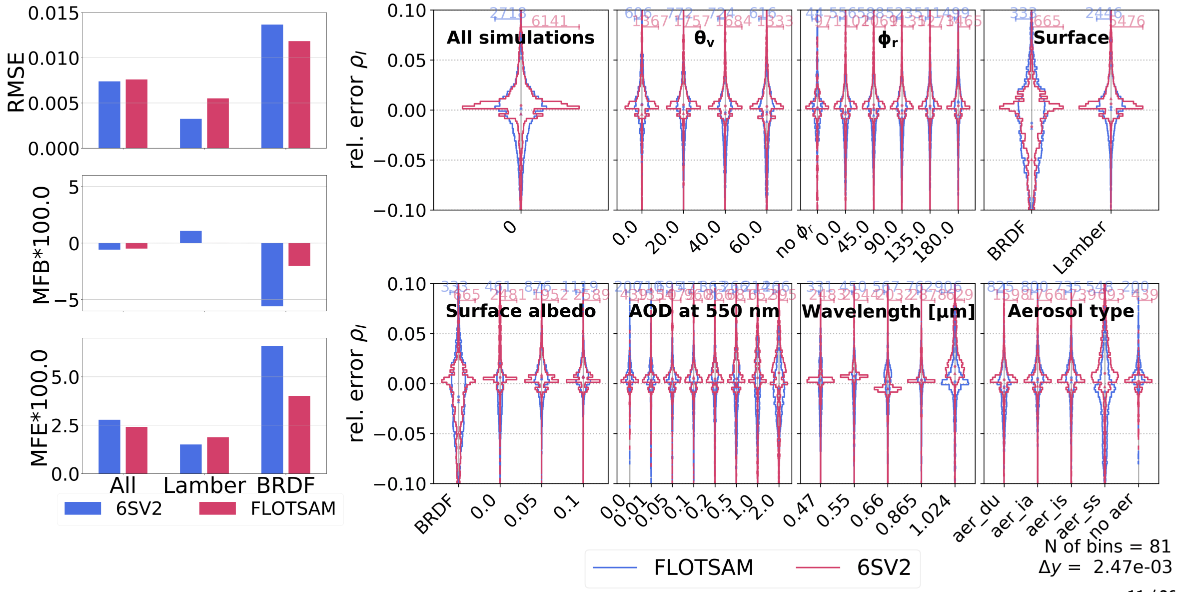
Results : VLIDORT reflectances



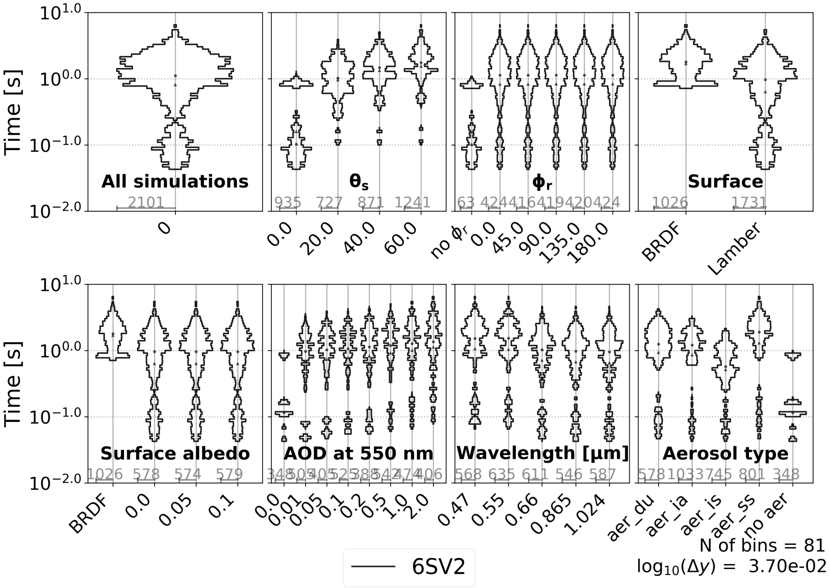
Results : Scalar VLIDORT and DISORT relative errors



Results : FLOTSAM and 6SV2 relative errors



Results : 6SV timing



Results : Time comparison [s]

		FLOTSAM	6SV2	DISORT
one-off set-up	Lambertian	2.87×10^{-5} (1.99×10^{-6})		
	BRDF	2.76 (5.28×10^{-3})		
ind	Lambertian	3.05×10^{-4} (1.84×10^{-6})	1.06 (0.87)	0.22 (0.18)
	BRDF	3.70×10^{-4} (1.49×10^{-5})	1.90 (0.95)	0.99 (0.18)
mult	Lambertian	9.90×10^{-2} (6.23×10^{-4})		0.29 (0.16)
	BRDF	9.96×10^{-2} (5.63×10^{-4})		1.21 (0.16)

FLOTSAM *mult* = 640 profiles ($0.1/640 \approx 0.15$ [ms])
6SV2 *mult* = 1 profile
DISORT *mult* = 20 profiles ($0.5/20 \approx 25$ [ms])

Summary of this part

- Benchmark has been designed for atmosphere with aerosols
- Target accuracy and computing time
- Tested with 4 models : VLIDORT, DISORT, FLOTSAM and 6SV2
- Errors in accuracy (against VLIDORT(V)) :
  - Lambertian MFE : 0.8, 1.5, 1.9 %
  - BRDF Cox-Munk MFE : 1.5, 6.6, 4 %
  - Spectral dependant (polarisation)
  - Aerosol optical depth dependant
  - Aerosol type dependant
- Computing time :
  - From seconds to less than milliseconds
  - Setup, single profile or multiple profile computations
  - Surface type dependence

Benchmark input data and VLIDORT(V) outputs are available at
`https://doi.org/10.5194/gmd-12-805-2019`

1D-Var short-wave reflectance assimilation in CAMS 43

Jerónimo Escribano [1], Olivier Boucher [5], Robin J. Hogan [4], Alessio Bozzo [2],Philippe Dubuisson [3], Johannes Flemming [4], Laurent Labonnote [3], Samuel Rémy [6] and Enza Di Tomaso [1] and Carlos Pérez García-Pando[1]

[1]Barcelona Supercomputing Center, Barcelona, Spain
[2]European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), Darmstadt, Germany
[3]European Centre for Medium Range Weather Forecasts, Reading, United Kingdom
[4]Laboratoire d'Optique Atmospherique, Université de Lille / CNRS, Villeneuve d'Ascq, France
[5]Institut Pierre-Simon Laplace, CNRS / Sorbonne Université, Paris, France
[6]HYGEOS, Lille, France

2 x AC science talks: Radiance assimilation for aerosols, ECMWF, 23/01/2020

Motivation

Interest in SW radiance assimilation

- Consistency of aerosol optical depth (AOD) retrievals with the model assumptions
- Use of prior information
- Better description of observational errors

Challenges

- Surface reflectance
- RTM accuracy and time
- Constraint of control variables by observations

Toy 1D-Var

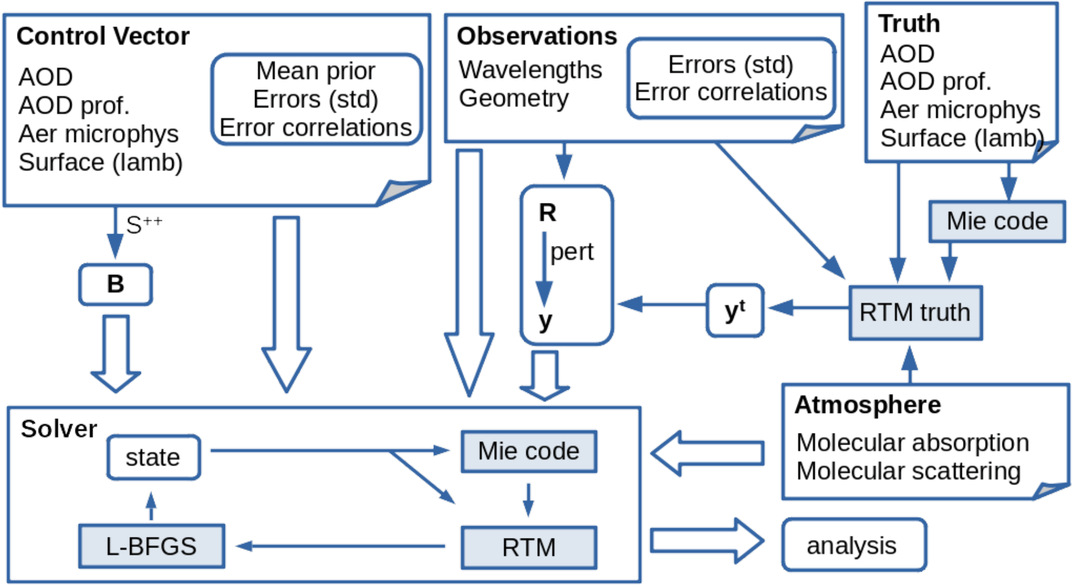
Implemented control vector

- AOD for each aerosol type, at a reference wavelength
- AOD of each layer (profile), for each aerosol type, at a reference wavelength
- Lambertian surface albedo for each wavelength
- Aerosol parameters:
  - Mode of the size distributions for externally and internally mixed aerosols
  - Standard deviation of the size distributions
  - Real and imaginary part of the refractive indices, for each wavelength
  - Proportion of number of particles of each mode of an internal and externally mixed distribution.

Observations

- Simulate true reflectances
- observations = true reflectances + ε, with $\varepsilon \sim N(0, \mathbf{R})$
- CDISORT RTM for the truth
- FLOTSAM RTM for the observation operator

Toy 1D-Var



Control Vector
AOD
AOD prof.
Aer microphys
Surface (lamb)
Mean prior
Errors (std)
Error correlations
Observations
Wavelengths
Geometry
Errors (std)
Error correlations
Truth
AOD
AOD prof.
Aer microphys
Surface (lamb)
S++
B
R
pert
y
Mie code
yt
RTM truth
Solver
state
Mie code
L-BFGS
RTM
Atmosphere
Molecular absorption
Molecular scattering
analysis

Test cases

- 4 wavelengths: 443, 550, 865 and 1024 nm
- 1 geometry: SZA: 0, VZA: 20, Azimuthal angle: 135, Scattering angle: 124.36 degrees.

Case 1

- Control : Sulfate AOD 550 nm
- Surface reflectance : truth

Case 3

- Control : Sulfate AOD 550 nm and surface refl.
- Surface reflectance error correlations of 0.6

Case 6

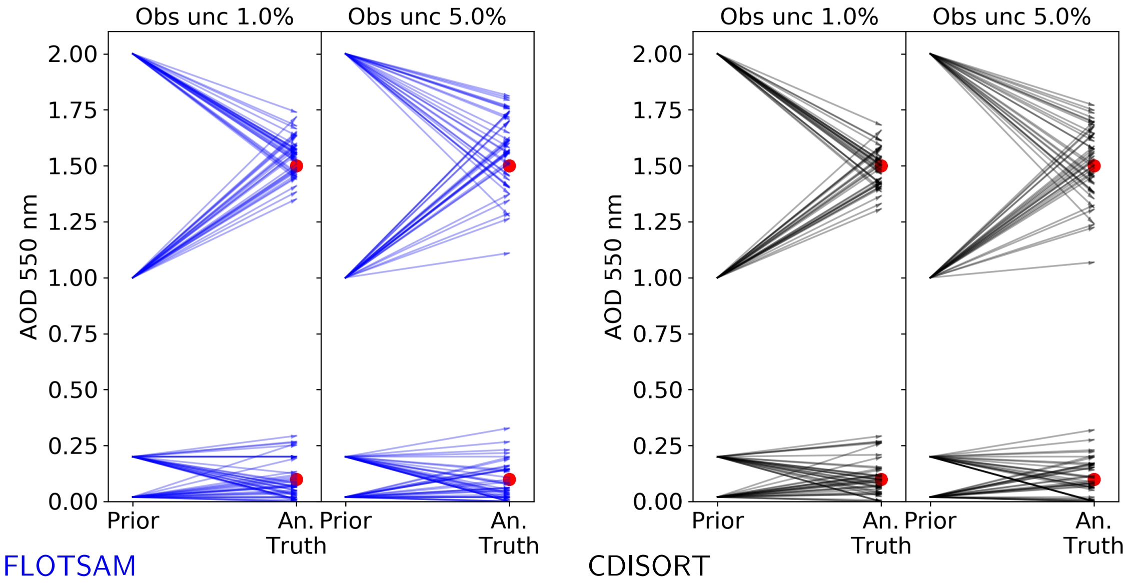
- Control : Organic matter AOD 550 nm and Sea salt AOD 550 nm.
- Surface reflectance: truth

Case 8

- Control : Dust profile AOD 550 nm
- Surface reflectance : truth

Case 1

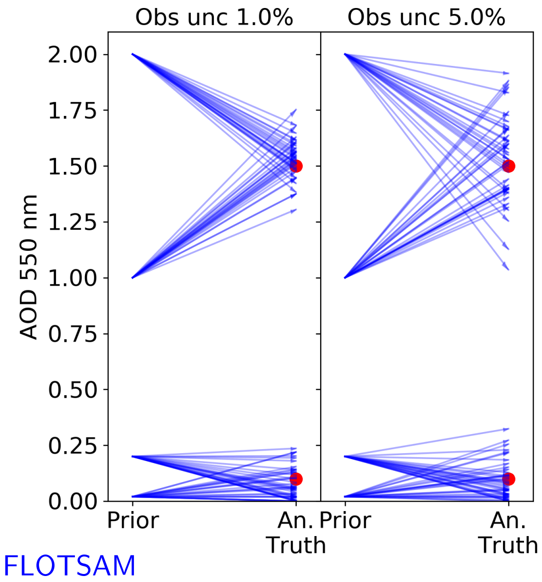
Sulfate AOD: truth 0.1 and 1.5; prior 0.02, 0.05, 1, 2

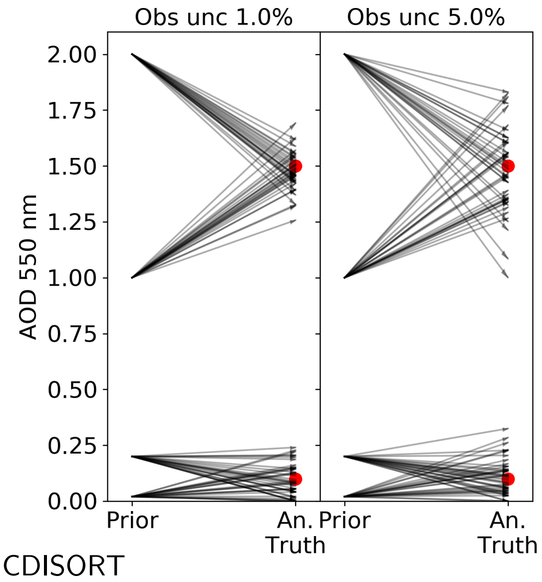


Case 3

Sulfate AOD: truth 0.1 and 1.5. Prior 0.02, 0.05, 1, 2

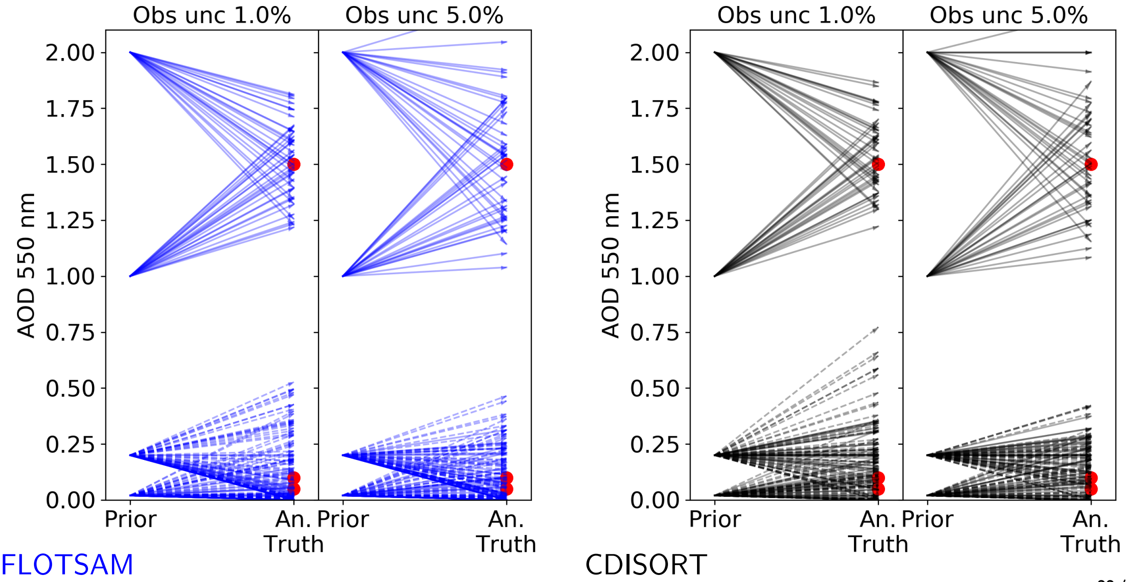
Surface reflectance : truth 0.3 all wavelengths. Prior : 0.36



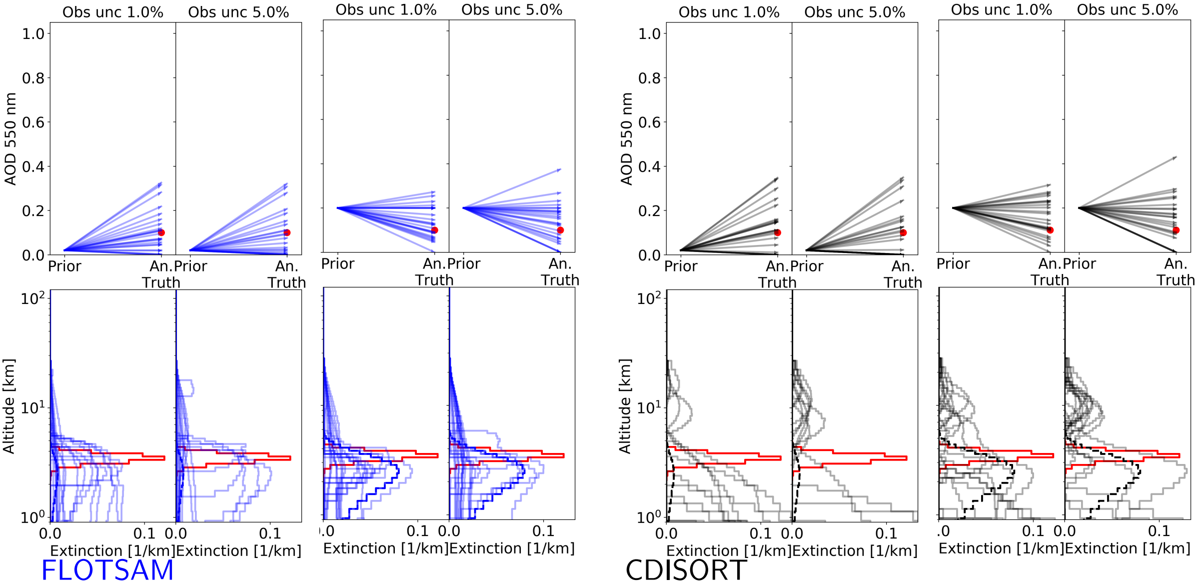


Case 6

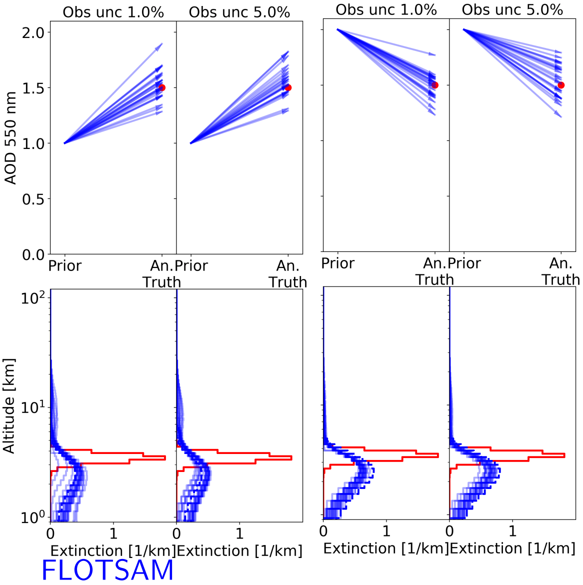
Organic matter (solid lines) AOD: truth 0.1 and 1.5. Prior 0.02, 0.2, 1, 2
Sea salt (dashed lines) AOD: truth 0.05 and 0.1. Prior 0.02, 0.2



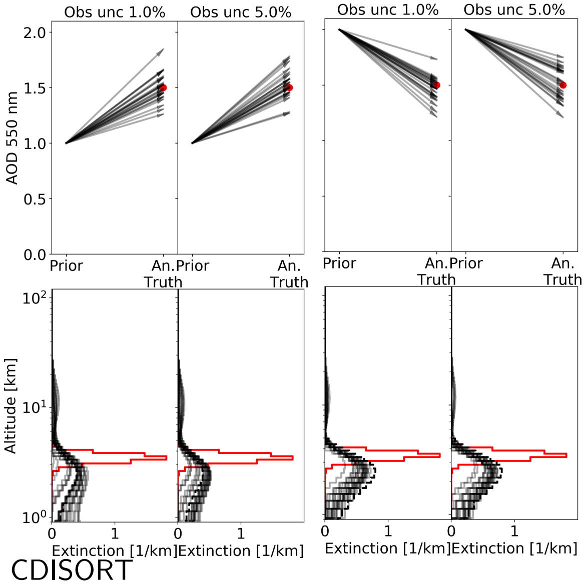
Case 8. AOD 0.1


Obs unc 1.0%
Obs unc 5.0%
AOD 550 nm
Prior
An.
Truth
Altitude [km]
Extinction [1/km]
FLOTSAM
CDISORT

Case 8 . AOD 1.5



Obs unc 1.0%
Obs unc 5.0%
Obs unc 1.0%
Obs unc 5.0%
AOD 550 nm
2.0
1.5
1.0
0.5
0.0
Prior
An.
Truth
Altitude [km]
10^2
10^1
10^0
0
1
Extinction [1/km]
FLOTSAM



Obs unc 1.0%
Obs unc 5.0%
Obs unc 1.0%
Obs unc 5.0%
AOD 550 nm
2.0
1.5
1.0
0.5
0.0
Prior
An.
Truth
Altitude [km]
10^2
10^1
10^0
0
1
Extinction [1/km]
CDISORT

Summary of this part

- Toy 1D-Var can be used to test configurations in the control vector and in the observations
- Similar analyses with FLOTSAM and CDISORT (truth: CDISORT)
- Analyses accuracy is better with less observational error (expected real reflectance accuracy of few percent)
- Not enough information (1 geometry, 4 wavelengths) to constraint profiles

Next steps:

- Select variables in the control vector
- Test with real observed reflectances
  - Surface, molecular absorption and scattering

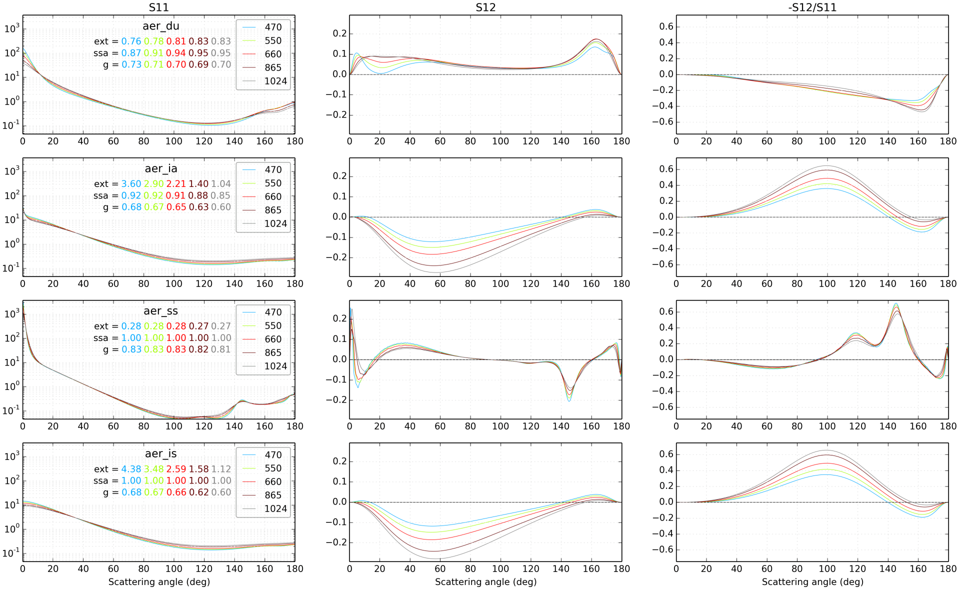
Thank you!

Questions?

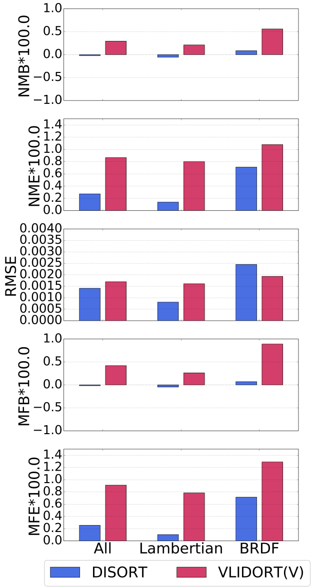
This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement H2020-MSCA-COFUND-2016-75443

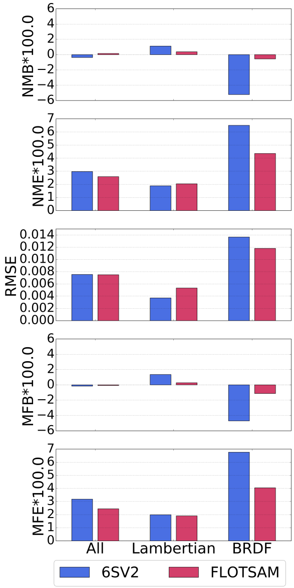
Extra slides

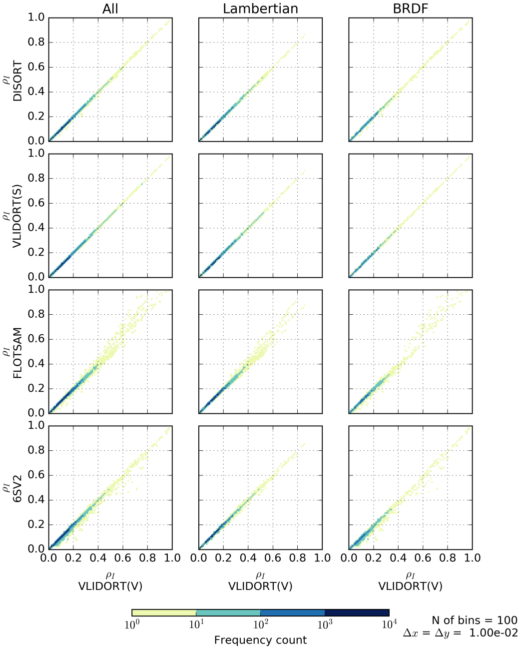
Aerosol types



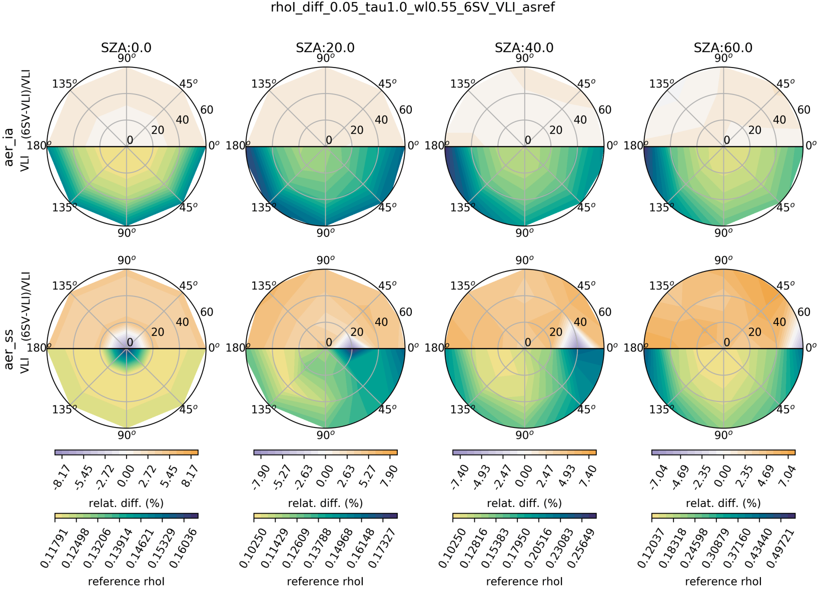
Metrics against VLIDORT(S)



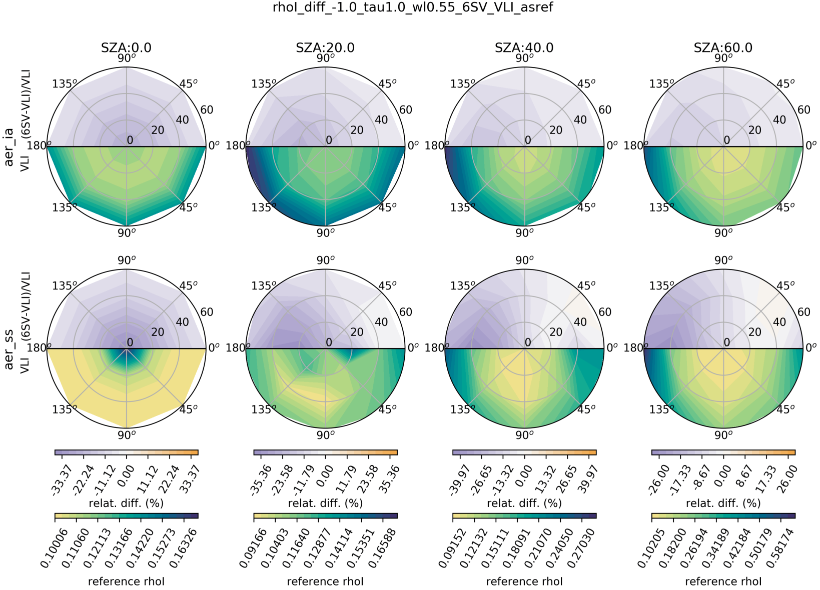



All
Lambertian
BRDF
ρ_I DISORT
ρ_I VLIDORT(S)
ρ_I FLOTSAM
ρ_I 6SV2
ρ_I VLIDORT(V)
ρ_I VLIDORT(V)
ρ_I VLIDORT(V)
Frequency count
N of bins = 100
$\Delta x = \Delta y =$ 1.00e-02

6SV2 - VLIDORT (V) , AOD=1 , 550 nm , Lambertian 0.05 , ind. abs. and sea salt



6SV2 - VLIDORT (V) , AOD=1 , 550 nm , CM BRDF, ind. abs. and sea salt



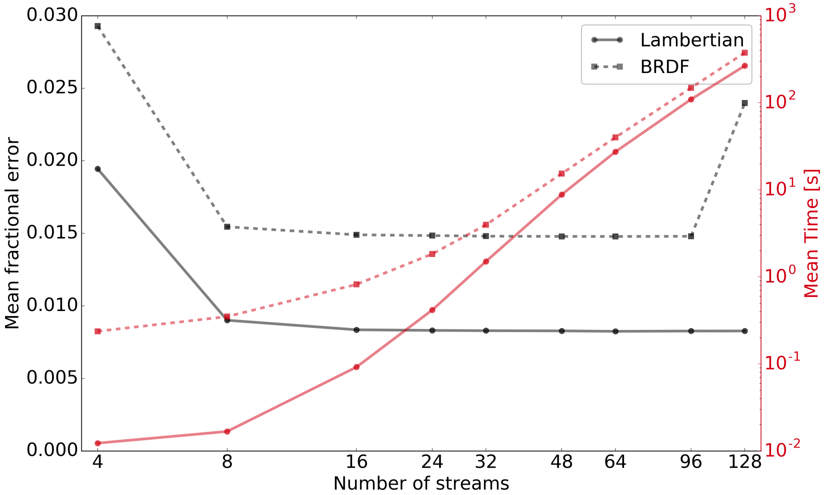
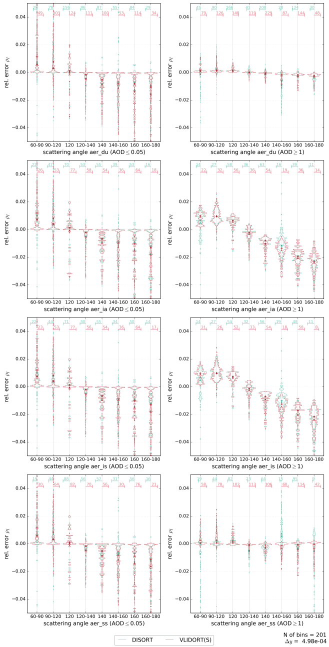
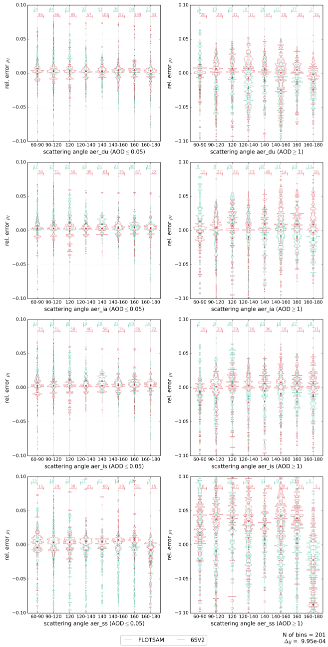


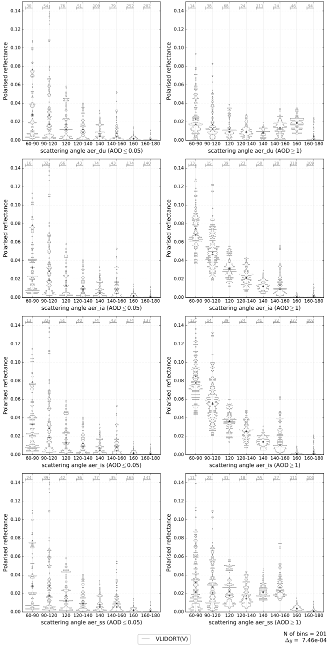
Figure: Accuracy (in black) and computing times (in red) for the DISORT model as a function of the number of streams used. The Lambertian and oceanic BRDF surface cases are shown with solid and dashed lines, respectively. The accuracy is shown in terms of Mean Fractional Error against VLIDORT (vector). The computing times are an average for 20 geometries and were estimated on a processor AMD Opteron 6378, 2.4 GHz.

	All		BRDF		Lambertian	
	DISORT	VLIDORT (scalar)	DISORT	VLIDORT (scalar)	DISORT	VLIDORT (scalar)
Reference (VLIDORT vector) Mean	0.114		0.108		0.116	
Model Mean	0.114	0.114	0.108	0.108	0.116	0.116
RMSE	0.002	0.002	0.003	0.002	0.002	0.002
Mean Fractional Bias (%)	–0.44	–0.42	–0.82	–0.89	–0.31	–0.26
Mean Fractional Error (%)	0.99	0.91	1.48	1.29	0.83	0.78
N	44,080	44,080	11,020	11,020	33,060	33,060
% of exps. with errors $>$ 0.5%	55.09	51.34	68.43	61.79	50.64	47.86
% of exps. with errors $>$ 1%	35.27	34.47	48.97	47.71	30.70	30.05
% of exps. with errors $>$ 2%	14.63	14.71	25.95	27.04	10.85	10.60
% of exps. with errors $>$ 2.5%	9.09	9.08	17.18	18.12	6.39	6.07
% of exps. with errors $>$ 5%	0.77	0.28	2.18	0.60	0.30	0.17
% of exps. with errors $>$ 7.5%	0.29	0.00	0.97	0.00	0.07	0.00
% of exps. with errors $>$ 10%	0.18	0.00	0.68	0.00	0.02	0.00

	All		BRDF		Lambertian	
	6SV2	FLOTSAM	6SV2	FLOTSAM	6SV2	FLOTSAM
Reference (VLIDORT vector) Mean	0.114		0.108		0.116	
Model Mean	0.114	0.114	0.102	0.107	0.117	0.116
RMSE	0.007	0.008	0.014	0.012	0.003	0.006
Mean Fractional Bias (%)	–0.58	–0.49	–5.60	–2.01	1.09	0.02
Mean Fractional Error (%)	2.78	2.41	6.60	4.01	1.51	1.88
N	44,080	44,080	11,020	11,020	33,060	33,060
% of exps. with errors $>$ 0.5%	71.30	80.21	82.56	89.86	67.54	77.00
% of exps. with errors $>$ 1%	45.84	63.70	71.08	79.76	37.42	58.35
% of exps. with errors $>$ 2%	30.04	39.91	54.44	61.91	21.91	32.58
% of exps. with errors $>$ 2.5%	25.04	32.02	48.57	53.80	17.20	24.76
% of exps. with errors $>$ 5%	14.01	11.89	34.50	26.05	7.18	7.17
% of exps. with errors $>$ 7.5%	8.25	4.70	26.00	11.59	2.34	2.40
% of exps. with errors $>$ 10%	5.63	1.97	20.20	5.56	0.77	0.77

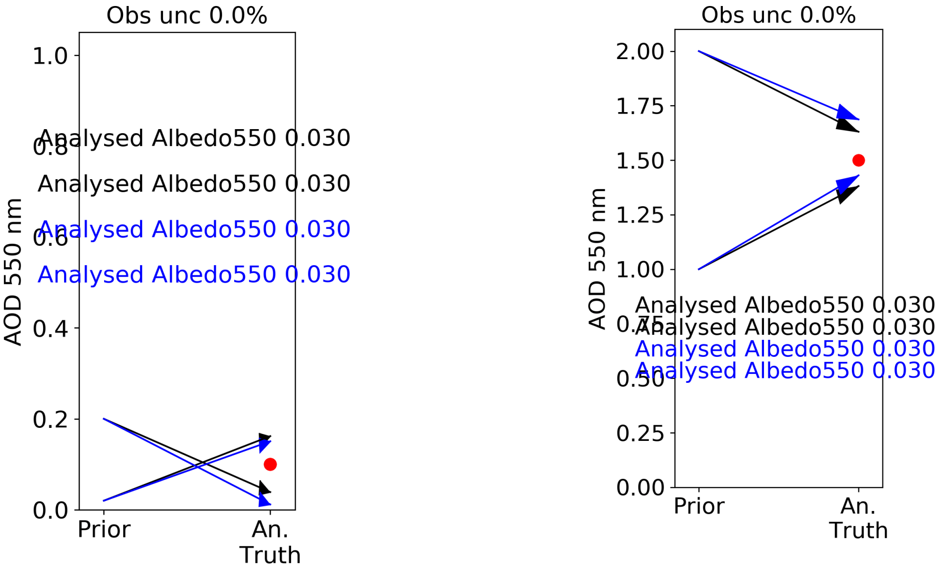

rel. error ρ_l
scattering angle aer_du (AOD ≤ 0.05)
scattering angle aer_du (AOD ≥ 1)
scattering angle aer_ia (AOD ≤ 0.05)
scattering angle aer_ia (AOD ≥ 1)
scattering angle aer_is (AOD ≤ 0.05)
scattering angle aer_is (AOD ≥ 1)
scattering angle aer_ss (AOD ≤ 0.05)
scattering angle aer_ss (AOD ≥ 1)
60-90 90-120 120 120-140 140 140-160 160 160-180
DISORT
VLIDORT(S)
N of bins = 201
Δy = 4.98e-04


rel. error ρ_l
60-90 90-120 120 120-140 140 140-160 160 160-180
scattering angle aer_du (AOD ≤ 0.05)
scattering angle aer_du (AOD ≥ 1)
scattering angle aer_ia (AOD ≤ 0.05)
scattering angle aer_ia (AOD ≥ 1)
scattering angle aer_is (AOD ≤ 0.05)
scattering angle aer_is (AOD ≥ 1)
scattering angle aer_ss (AOD ≤ 0.05)
scattering angle aer_ss (AOD ≥ 1)
FLOTSAM
6SV2
N of bins = 201
Δy = 9.95e-04


Polarised reflectance
scattering angle aer_du (AOD ≤ 0.05)
scattering angle aer_du (AOD ≥ 1)
scattering angle aer_ia (AOD ≤ 0.05)
scattering angle aer_ia (AOD ≥ 1)
scattering angle aer_is (AOD ≤ 0.05)
scattering angle aer_is (AOD ≥ 1)
scattering angle aer_ss (AOD ≤ 0.05)
scattering angle aer_ss (AOD ≥ 1)
60-90 90-120 120 120-140 140 140-160 160 160-180
VLIDORT(V)
N of bins = 201
Δy = 7.46e-04

Case 1

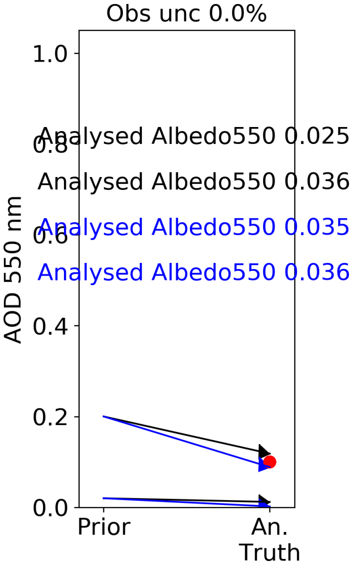
Sulfate AOD: truth 0.1 and 1.5; prior 0.02, 0.05, 1, 2

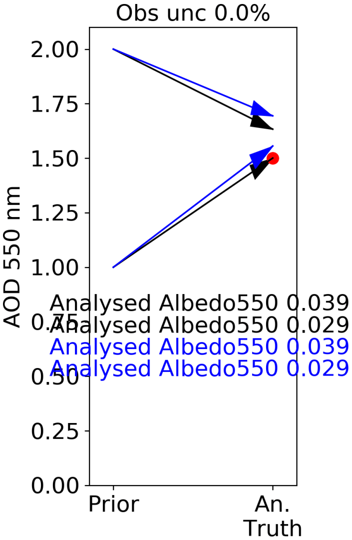


Case 3

Sulfate AOD: truth 0.1 and 1.5. Prior 0.02, 0.05, 1, 2

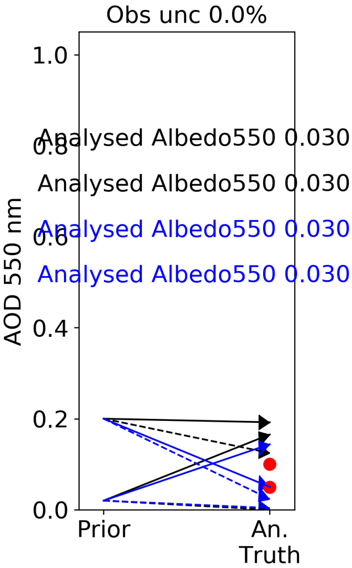
Surface reflectance : truth 0.3 all wavelengths. Prior : 0.36

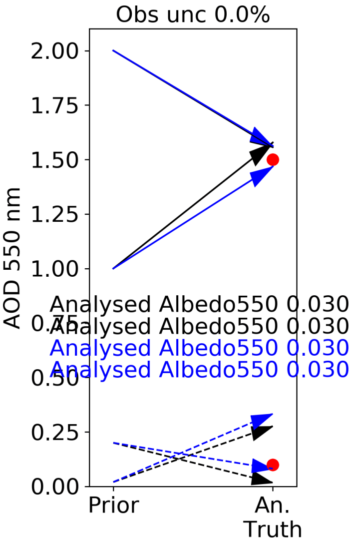




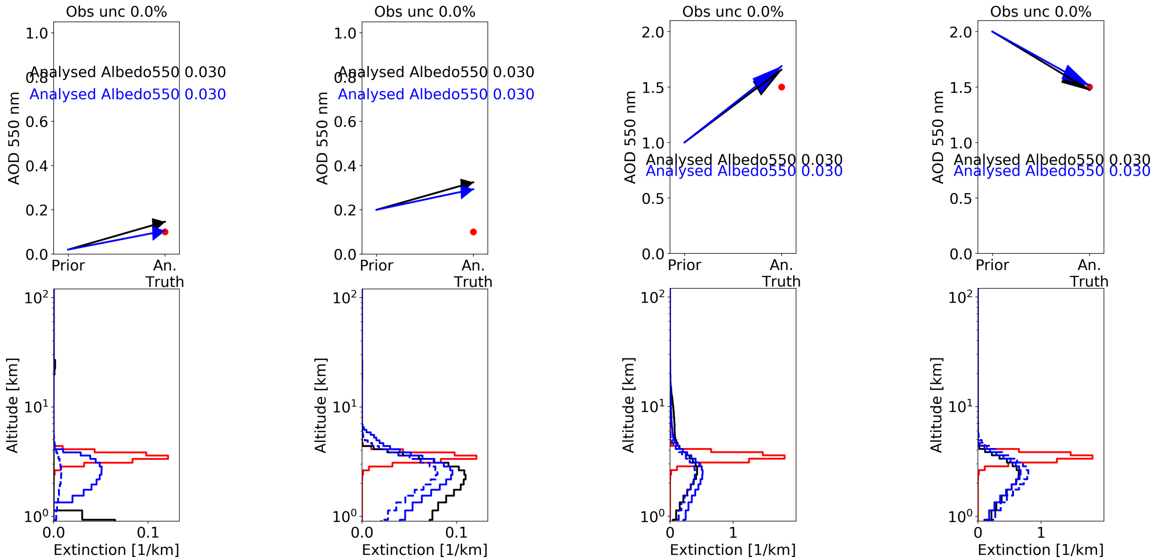
Case 6

Organic matter (solid lines) AOD: truth 0.1 and 1.5. Prior 0.02, 0.2, 1, 2
Sea salt (dashed lines) AOD: truth 0.05 and 0.1. Prior 0.02, 0.2





Case 8


Obs unc 0.0%
Analysed Albedo550 0.030
Analysed Albedo550 0.030
AOD 550 nm
Prior
An.
Truth
Altitude [km]
Extinction [1/km]
Obs unc 0.0%
Analysed Albedo550 0.030
Analysed Albedo550 0.030
AOD 550 nm
Prior
An.
Truth
Altitude [km]
Extinction [1/km]
Obs unc 0.0%
Analysed Albedo550 0.030
Analysed Albedo550 0.030
AOD 550 nm
Prior
An.
Truth
Altitude [km]
Extinction [1/km]
Obs unc 0.0%
Analysed Albedo550 0.030
Analysed Albedo550 0.030
AOD 550 nm
Prior
An.
Truth
Altitude [km]
Extinction [1/km]

AOD and reflectance at TOA 550 nm