Investigation of 3D-effects for satellite observations of volcanic plumes

Thomas Wagner (1), Simon Warnach (1), **Steffen Beirle** (1), Nicole Bobrowski (2,3), Adrian Jost (1) Tjarda Roberts (4), and Luke Surl (5,6)

Postcard from measurement campaign in Mexico city 2005

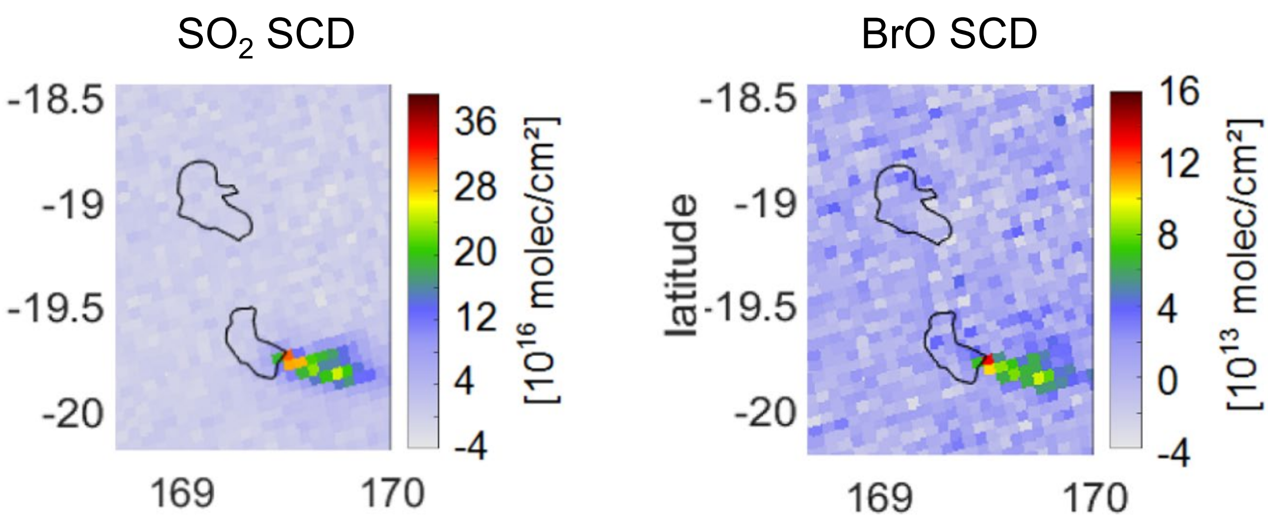
(1) Max Planck Institute for Chemistry, Germany
(2) Institute of Environmental Physics, University of Heidelberg, Heidelberg, Germany
(3) Istituto Nazionale Geofisica e Vulcanologia Catania, Italy
(4) Laboratoire de Physique et de Chimie de l'Environnement et de l'Espace, CNRS, Université d'Orléans, Orléans, France
(5) LATMOS/IPSL, Sorbonne Université, UVSQ, CNRS, Paris, France
(6) Department of Chemistry, University of Aberdeen, Aberdeen, UK

Motivation / Outline:

Why are 3D effects important?

- pixel size of TROPOMI is smaller than the height of the troposphere and photon path lengths in the UV/vis
- volcanic plumes have dimensions similar to or smaller than the pixel size of TROPOMI (3.5 x 5.5 km²)

→ 3D effects become increasingly important



Mount Yasur 2020-06-24

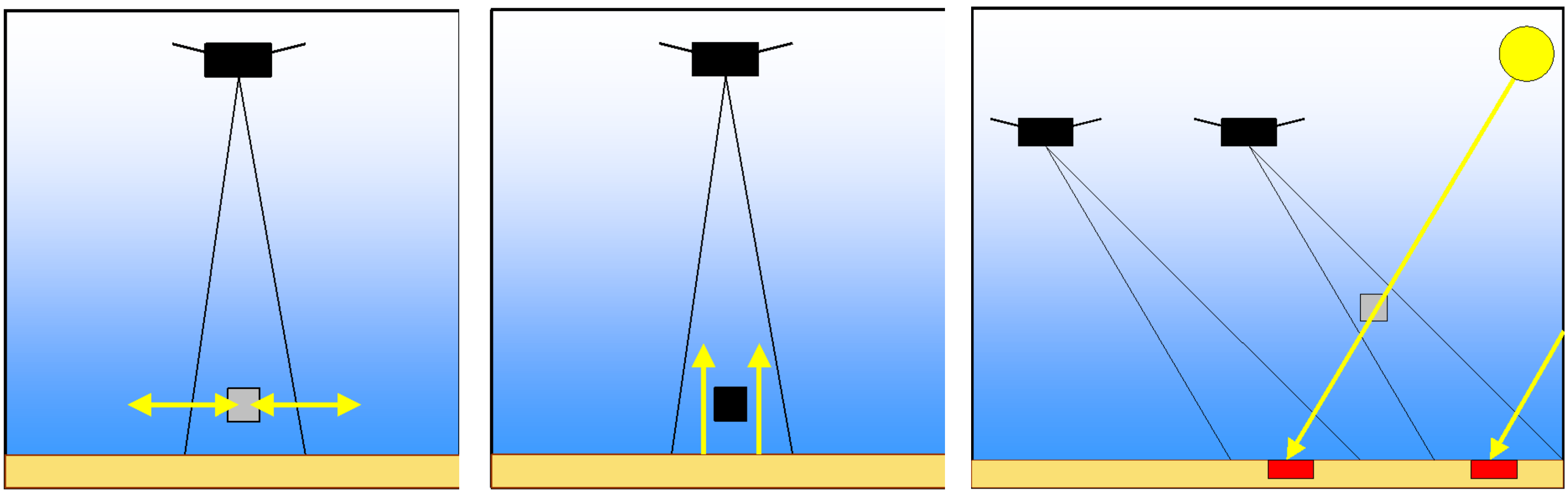
Figures from S. Warnach

- so far, horizontally homogenous assumptions (1D-AMFs) are used for analysis of volcanic plumes
  → how important are 3D effects on satellite retrievals?

Motivation / Outline:

Most important 3D effects:

1. effect of horizontal light paths
2. saturation effects (SO_2)
3. geometrical effects (SZA, VZA) for elevated plumes
4. side scattering effects (not included in this presentation)



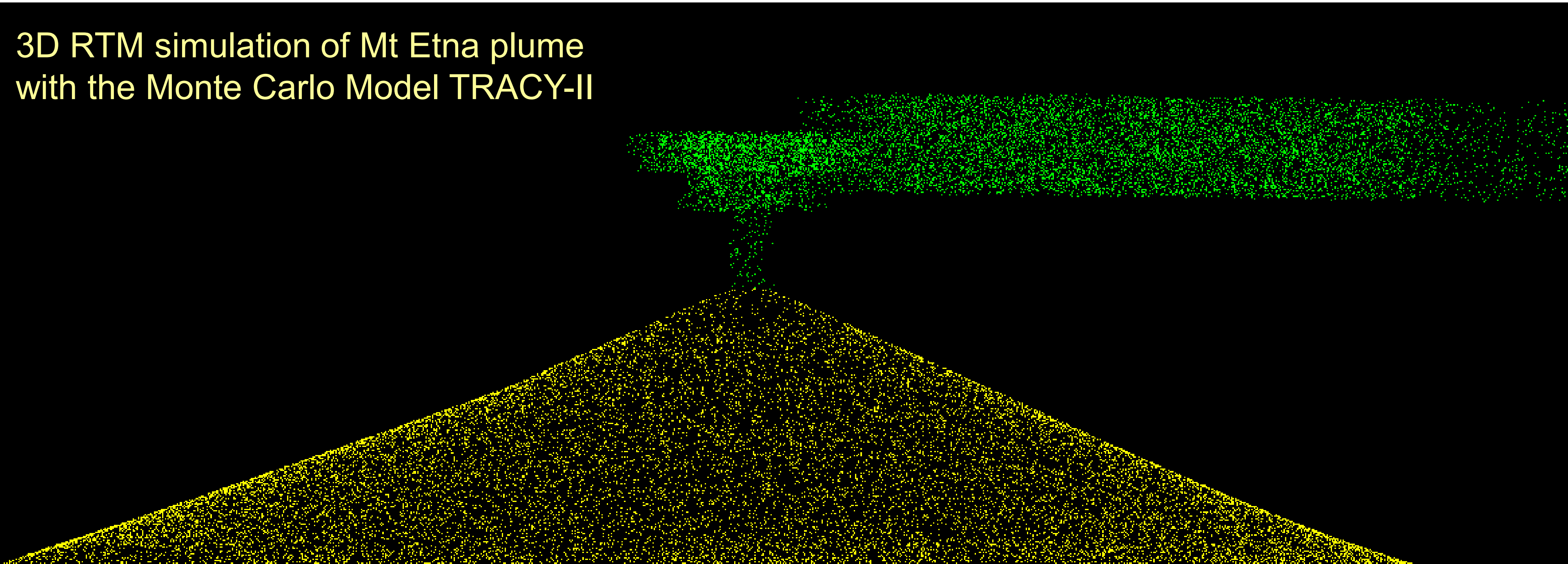
3D Monte-Carlo RTM simulations (TRACY-2)

Developed by Tim Deutschmann, Uni-Heidelberg (see Wagner et al., ACP, 2007)

- 3D-distributions of trace gases and aerosols
- suface topography

RTM set up

- volcanic plumes at different altitudes with different horizontal extensions (0.2 km – 222 km)
- wavelenths: 313 (SO_2), 340 (BrO), 440 nm (IO, SO_2, H_2O)
- FOV: TROPOMI (3.5x5.5km²), OMI, SCIA, GOME-2, 200x200 km²



Trace gas and aerosol scenarios

Scenario	VCDs for 1 km plume
BrO VCD_{low} ($1 \cdot 10^{13}$ molec/cm²)	100
BrO VCD_{high} ($1 \cdot 10^{13}$ molec/cm²)	1000
IO VCD_{low} ($1 \cdot 10^{13}$ molec/cm²)	50
IO VCD_{high} ($1 \cdot 10^{13}$ molec/cm²)	500
SO_2 $VCD_{weak, low}$ ($1 \cdot 10^{17}$ molec/cm²)	4
SO_2 $VCD_{weak, high}$ ($1 \cdot 10^{17}$ molec/cm²)	40
SO_2 $VCD_{strong, 1}$ ($1 \cdot 10^{17}$ molec/cm²)	100
SO_2 $VCD_{strong, 2}$ ($1 \cdot 10^{17}$ molec/cm²)	250
SO_2 $VCD_{strong, 3}$ ($1 \cdot 10^{17}$ molec/cm²)	1000
SO_2 $VCD_{strong, 4}$ ($1 \cdot 10^{17}$ molec/cm²)	4000

weak absorbers

strong absorbers

The trace gas VCDs are given for a 1 x 1 x 1 km³ plume.

They are derived from ground based observations

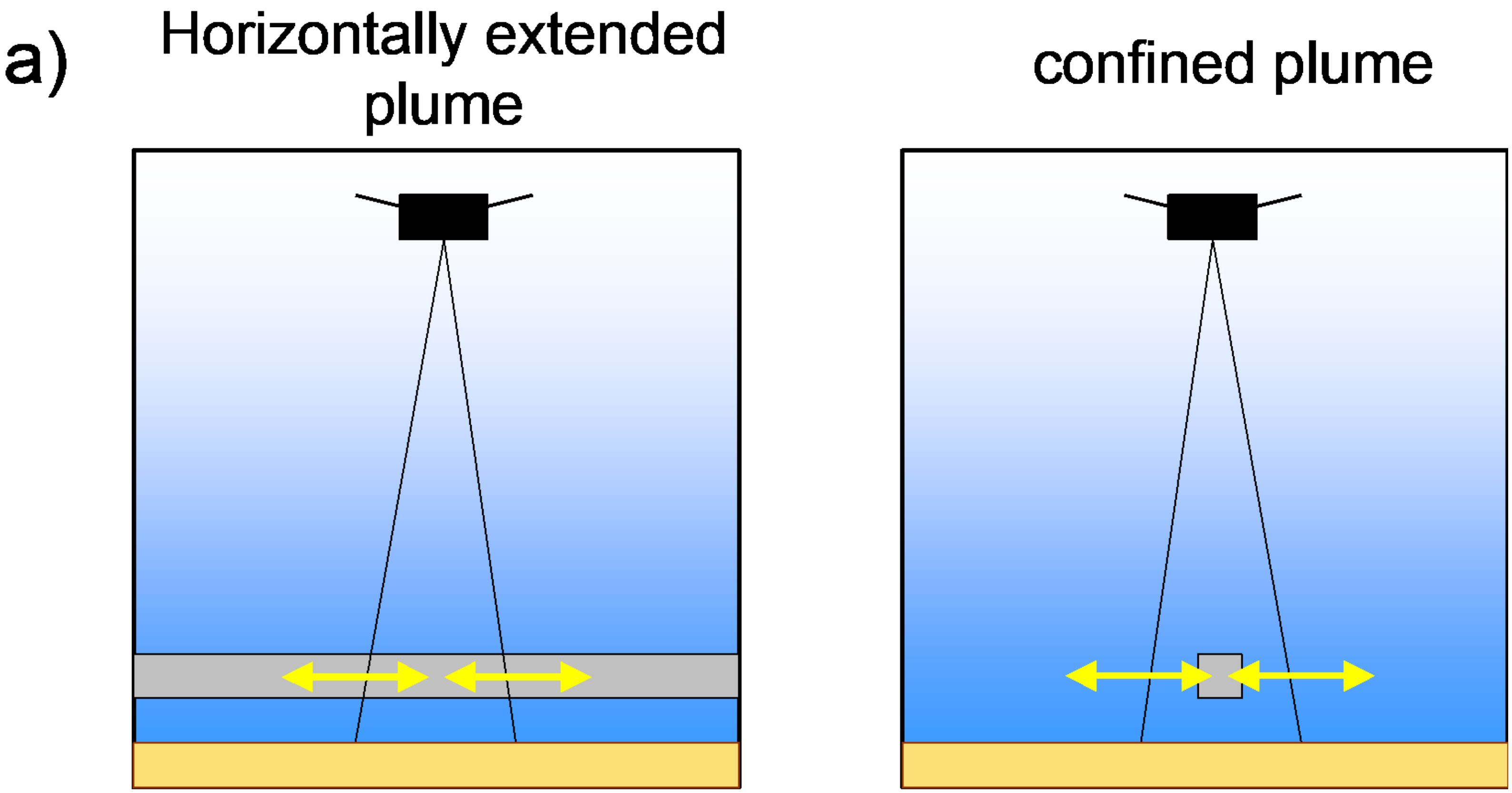
The amount of molecules / aerosols is kept constant for the different plume extensions

Trace gas and aerosol scenarios

The amount of molecules / aerosols is kept constant for the different plume extensions

Scenario	Trace gas VCDs for different horizontal plume extension								
	1 km	2 km	4 km	6 km	10 km	14 km	20 km	30 km	40 km
BrO VCD_{low} ($1 \cdot 10^{13}$molec/cm²)	100	25	6.25	2.78	1	0.51	0.25	0.11	0.06
BrO VCD_{high} ($1 \cdot 10^{13}$molec/cm²)	1000	250	62.5	27.8	10	5.10	2.5	1.11	0.63
IO VCD_{low} ($1 \cdot 10^{13}$molec/cm²)	50	12.5	3.13	1.39	0.5	0.26	0.13	0.06	0.03
IO VCD_{high} ($1 \cdot 10^{13}$molec/cm²)	500	125	31.3	13.9	5	2.55	1.25	0.56	0.31
SO_2 $VCD_{weak, low}$ ($1 \cdot 10^{17}$molec/cm²)	4	1	0.25	0.11	0.04	0.02	0.01	0.004	0.003
SO_2 $VCD_{weak, high}$ ($1 \cdot 10^{17}$molec/cm²)	40	10	2.5	1.1	0.4	0.20	0.1	0.044	0.03
SO_2 $VCD_{strong, 1}$ ($1 \cdot 10^{17}$molec/cm²)	100	25	6.25	2.78	1	0.51	0.25	0.11	0.06
SO_2 $VCD_{strong, 2}$ ($1 \cdot 10^{17}$molec/cm²)	250	62.5	15.6	6.9	2.5	1.28	0.63	0.28	0.16
SO_2 $VCD_{strong, 3}$ ($1 \cdot 10^{17}$molec/cm²)	1000	250	62.5	27.8	10	5.10	2.50	1.11	0.63
SO_2 $VCD_{strong, 4}$ ($1 \cdot 10^{17}$molec/cm²)	4000	1000	250	111	40	20.4	10	4.44	2.5

1. Effect of horizontal light paths

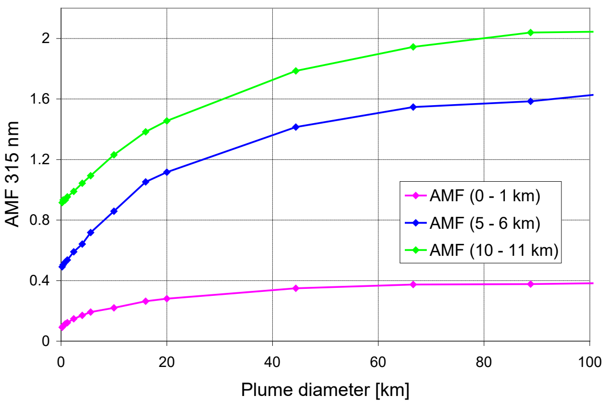


Horizontal light paths contain trace gas absorption from outside the ground pixel

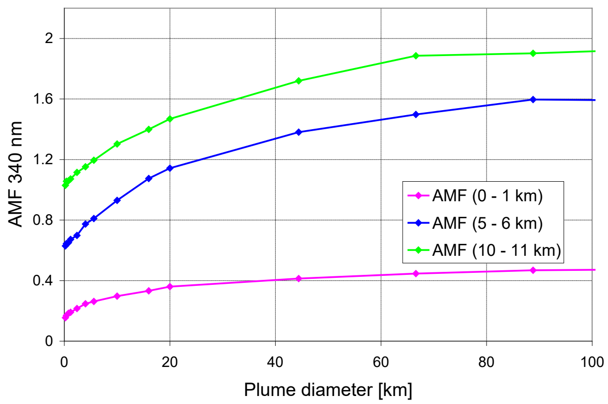
Dependence on horizontal plume extension

AMFs for nadir view, SZA = 0°, different plume heights

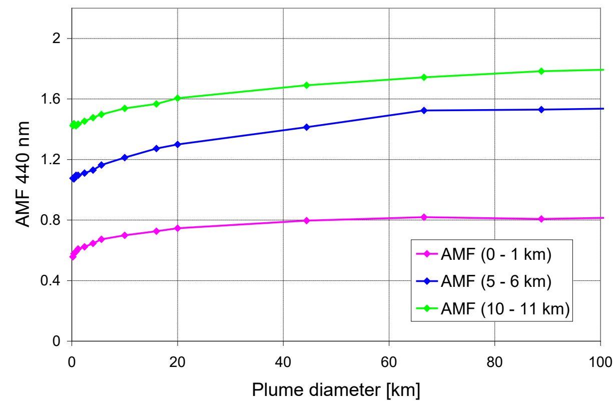
313 nm

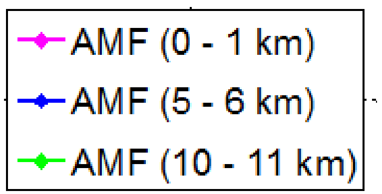


340 nm



440 nm





The AMFs depend strongly on the horizontal plume extension

Plume scan

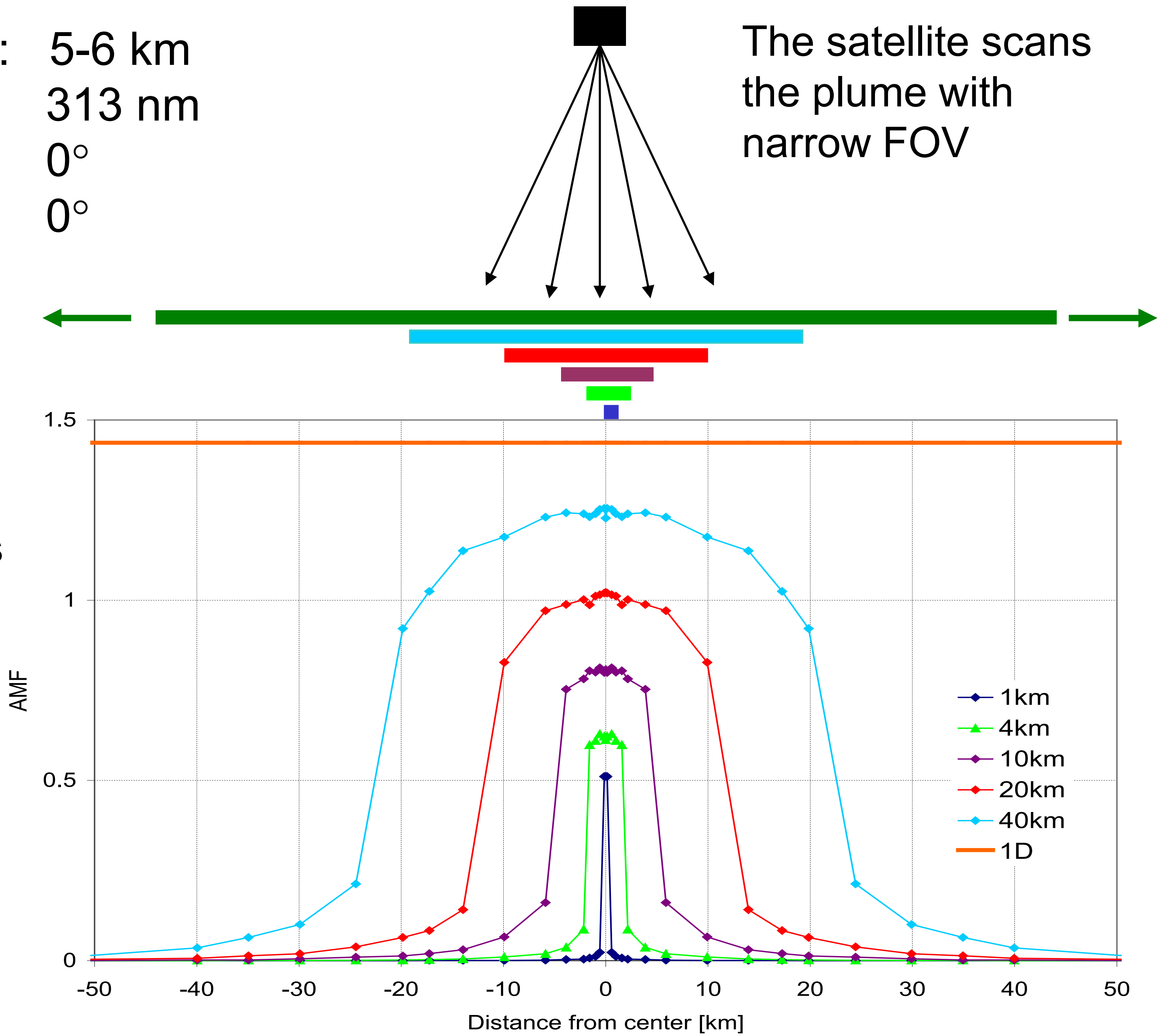
Plume altitude: 5-6 km

Wavelength: 313 nm

SZA: 0°

VZA: 0°

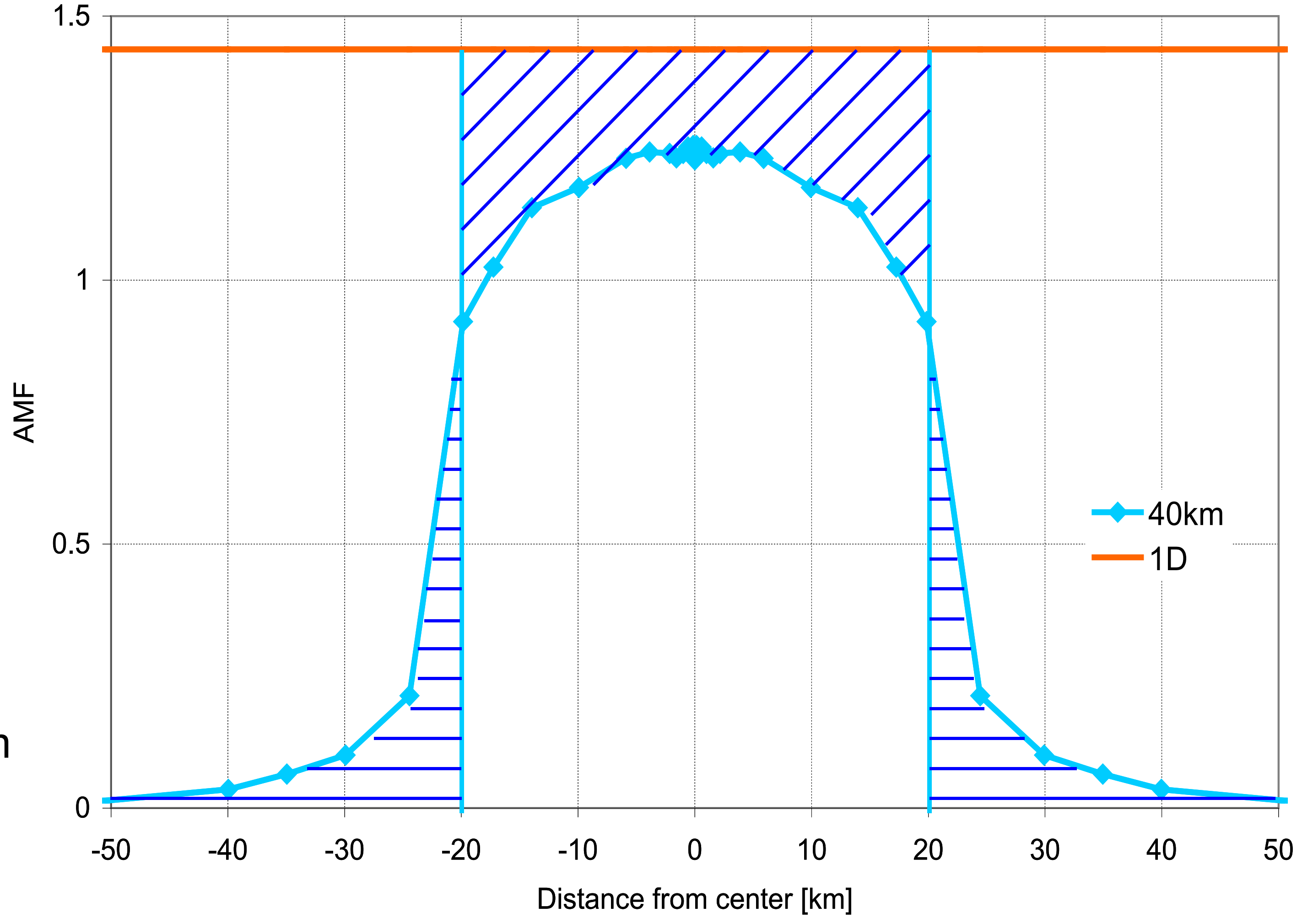
The satellite scans the plume with narrow FOV



=> for narrow plumes the AMFs are strongly reduced

=> there are no sharp edges

- what does this mean for quantitative estimates?
- can increased AMF ‚outside‘ the plume compensate for decrease ‚inside‘ the plume? (in both horizontal dimensions)



altitude: 5 - 6 km
Wavelength: 313 nm
SZA: 0°
VZA: 0°

Example for TROPOMI observations of a 1 x 1 x 1 km^3 plume at 5 – 6 km altitude (313 nm, SO_2 VCD: 1 · 10^{18} molec/cm²)

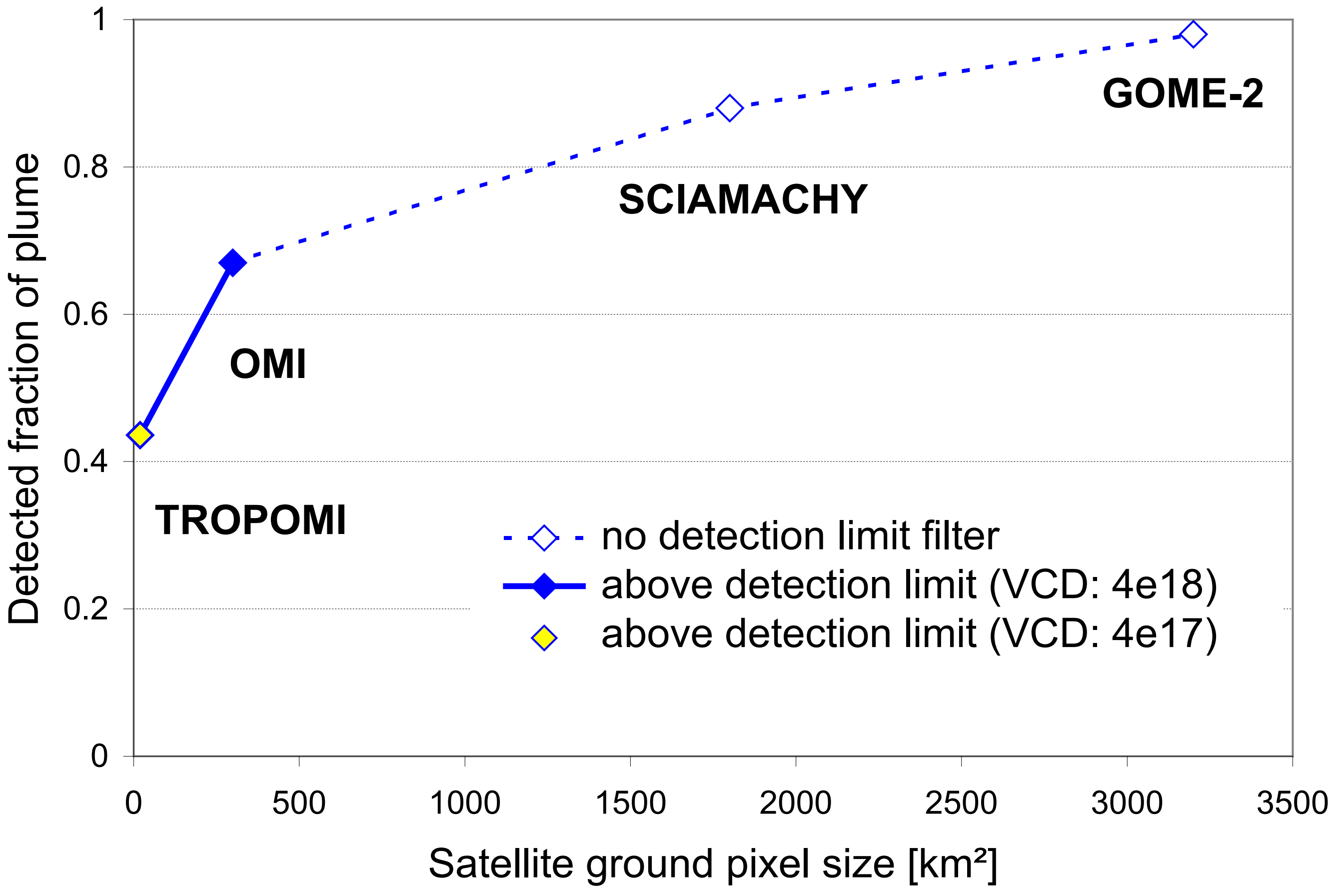
0.9% <0.001	1.5% <0.001	2.1% <0.001	1.5% <0.001	0.9% <0.001
1.3% <0.001	3.2% <0.001	43.6% 0.013	3.2% <0.001	1.3% <0.001
0.9% <0.001	1.5% <0.001	2.1% <0.001	1.5% <0.001	0.9% <0.001

fraction of plume amount

optical depth

Red colours indicate measurements above the detection limit

Observations of different instruments of a 1 x 1 x 1 km^3 plume at 5 – 6 km altitude (SO_2 at 313 nm)



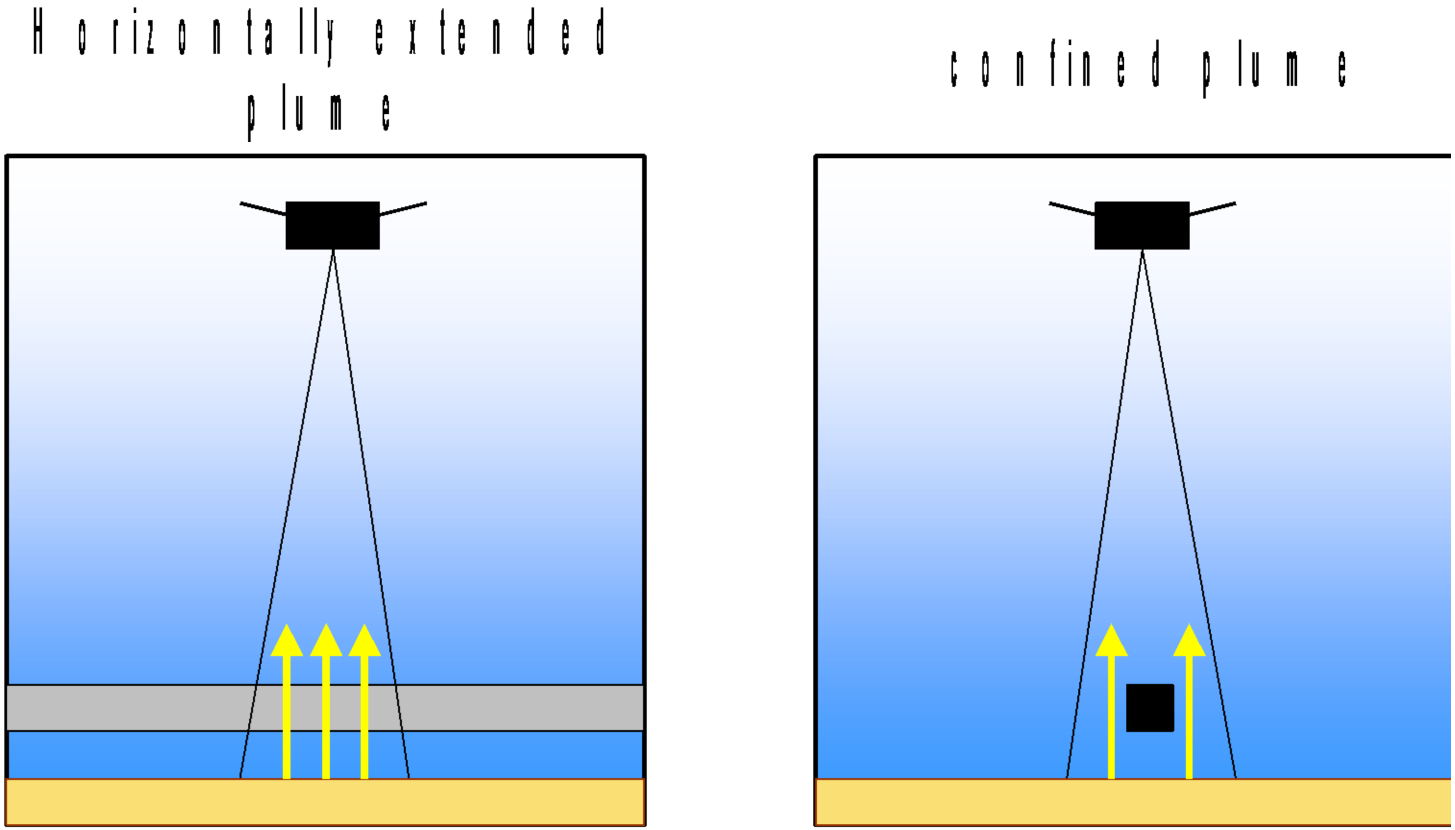
The full blue (yellow) symbols indicate observations above the detection limit for a high (low) trace gas VCD

=> narrow plumes can only be observed from instruments with high spatial resolution

=> But for such observations, the effect of horizontal lights paths is strongest

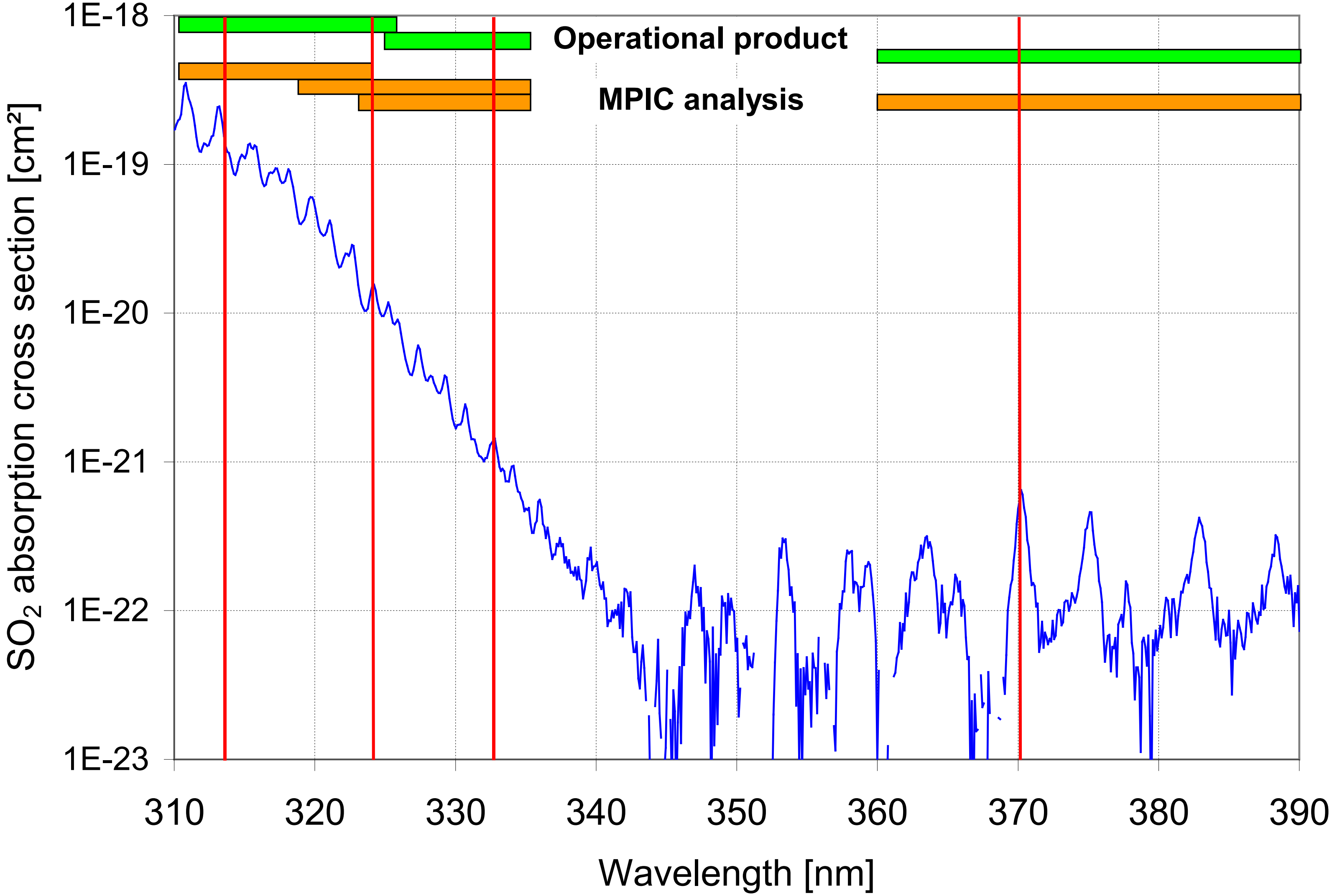
2. Saturation effect

b)



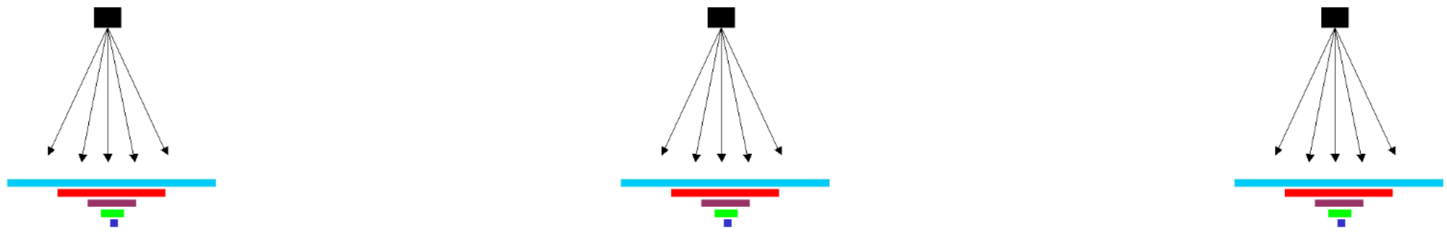
Extreme case: for narrow plumes (right), no light is received from the plume (strong absorption), and the light from outside the plume has seen no absorption

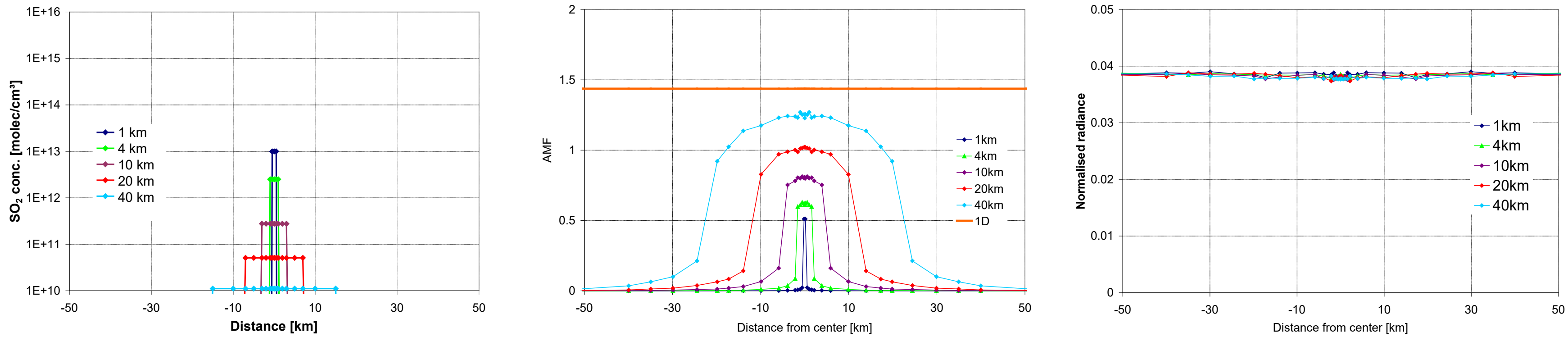
Saturation effect



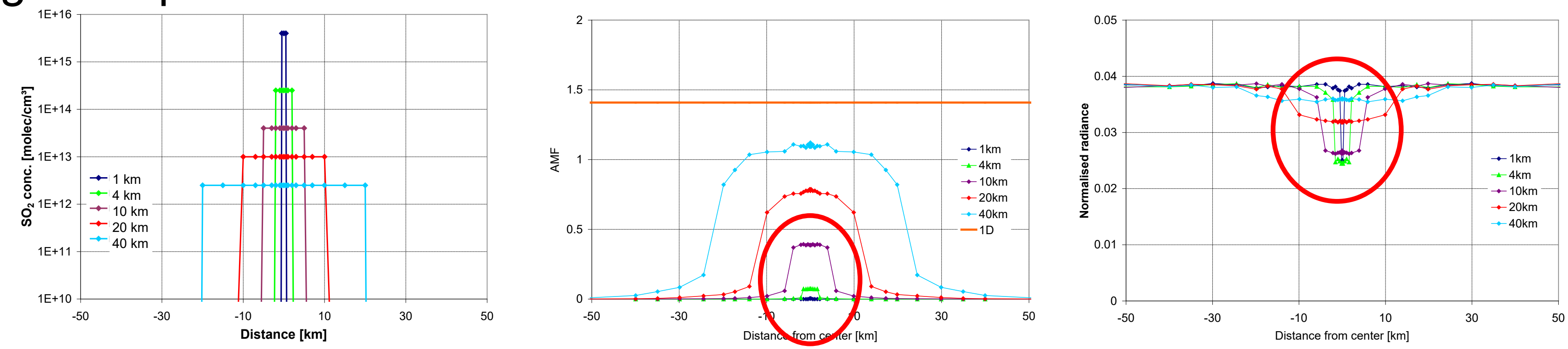
Green / orange bars: spectral ranges used for SO_2 analyses
Red vertical lines: wavelenghts used in this study

weak absorption





strong absorption



Note: the same amount of molecules is present in all plumes (with different horizontal extensions, see different colours)

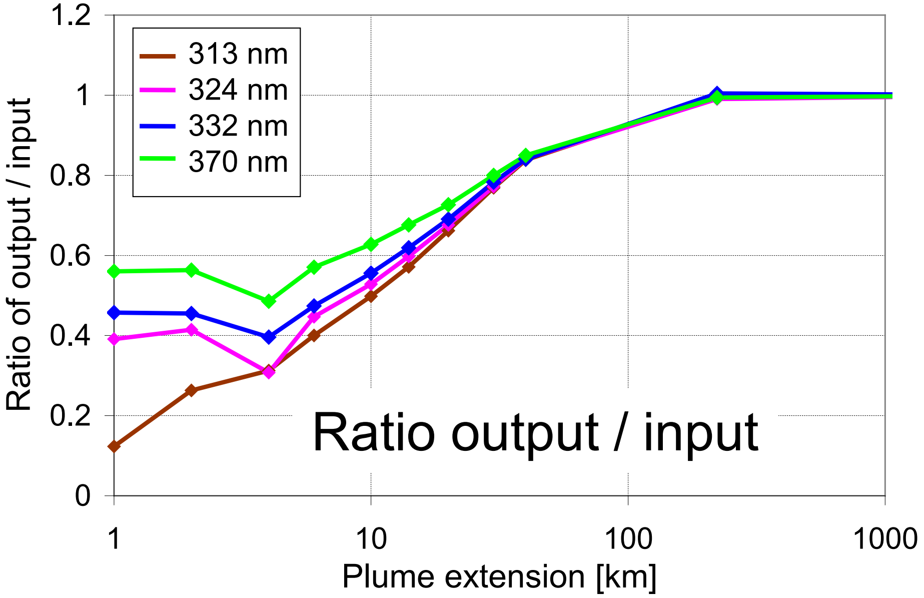
Two effects of strong absorption:

a) AMF becomes smaller; b) radiance becomes smaller

Saturation effect (medium strong absorption)

TROPOMI observations at different wavelengths

($VCD_{ref} = 1 \times 10^{19}$ molec/cm²)



Red line indicates the threshold for the switch from standard fit window to alternative fit windows

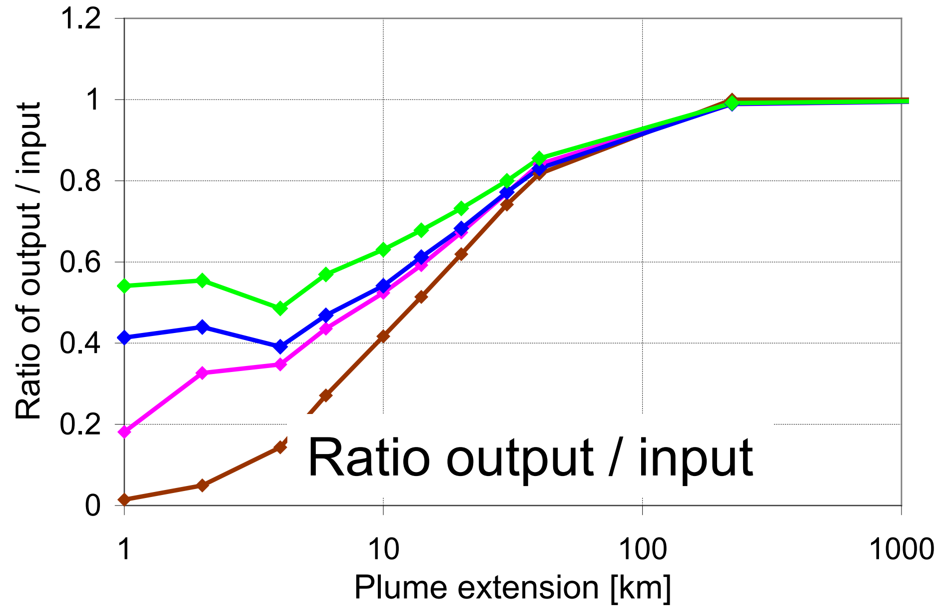
SCD

From results in standard fit window alone, no switch to alternative fit window will be initiated.

Saturation effect (very strong absorption)

TROPOMI observations at different wavelengths

(VCD_{ref} = 1 ×10^{20} molec/cm²)



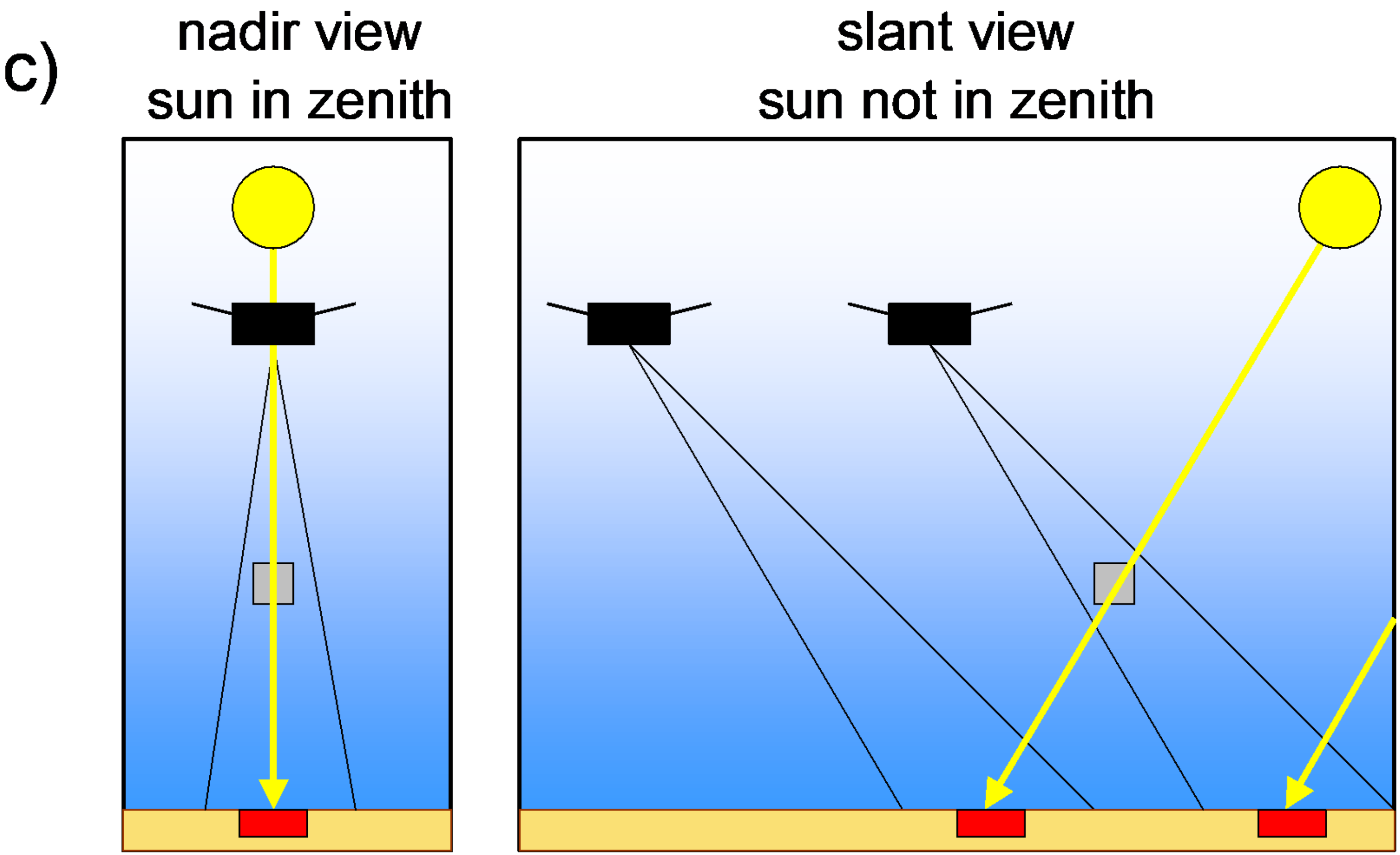
SCD

Red line indicates the threshold for the switch from standard fit window to alternative fit windows

From results in standard fit window alone, no switch to alternative fit window will be initiated

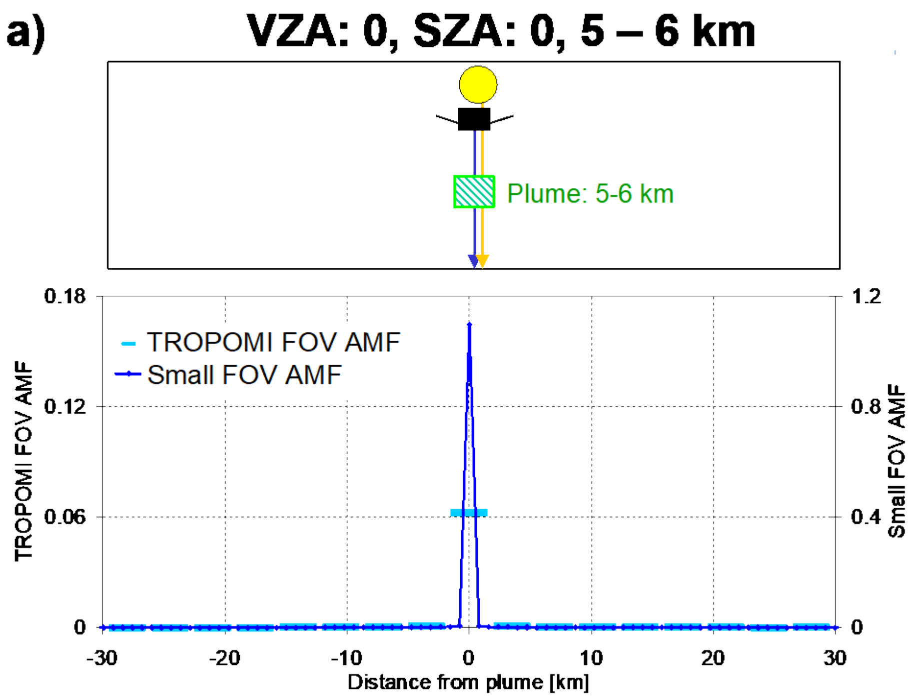
Recommendation: always analyse SO_2 simultaneously in different fit windows

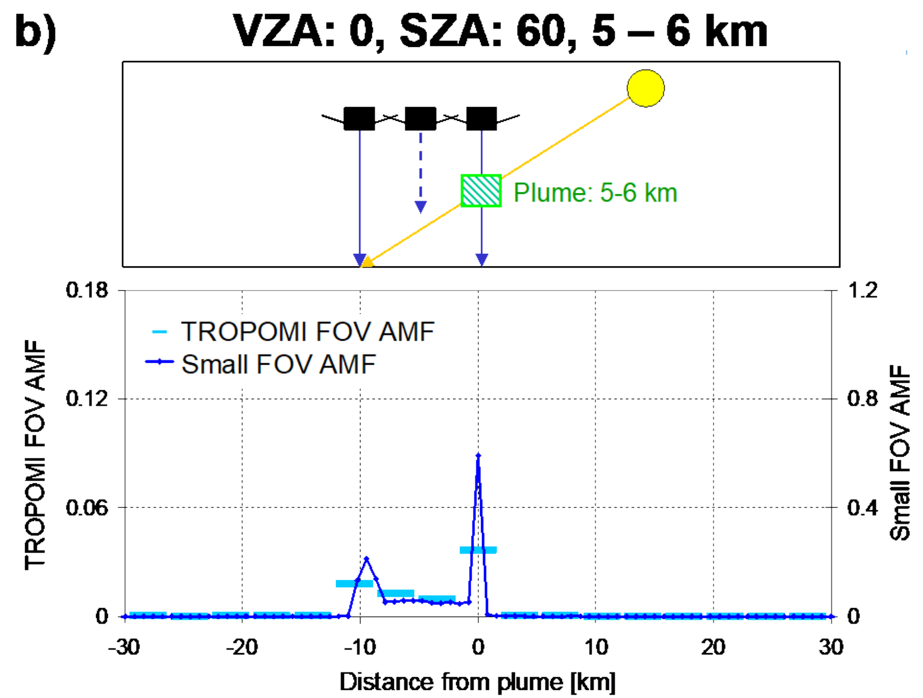
3. Geometric effects



Location of ground pixel(s) seeing the plume and location of the plume are usually not the same (for elevated plumes)

Geometric effects

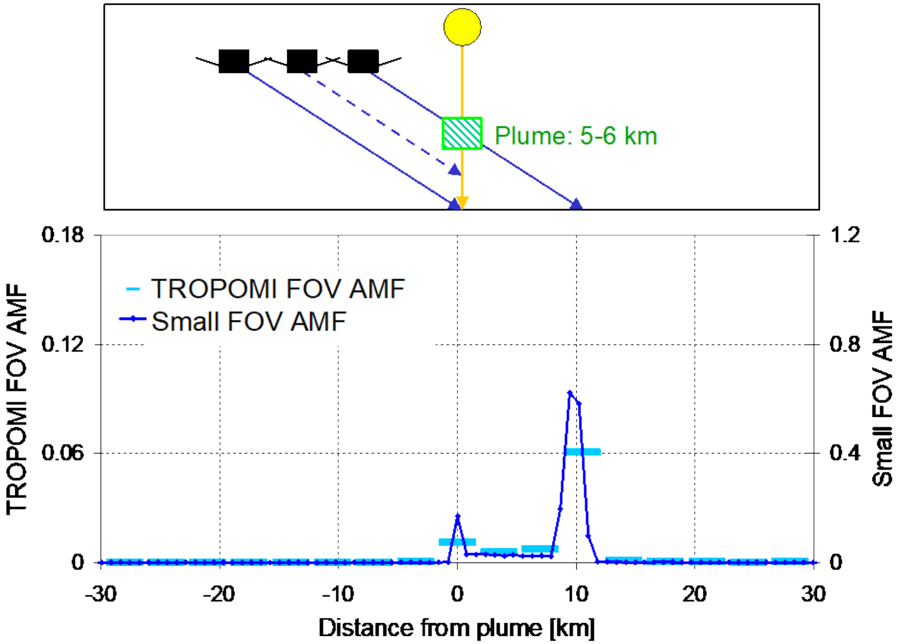




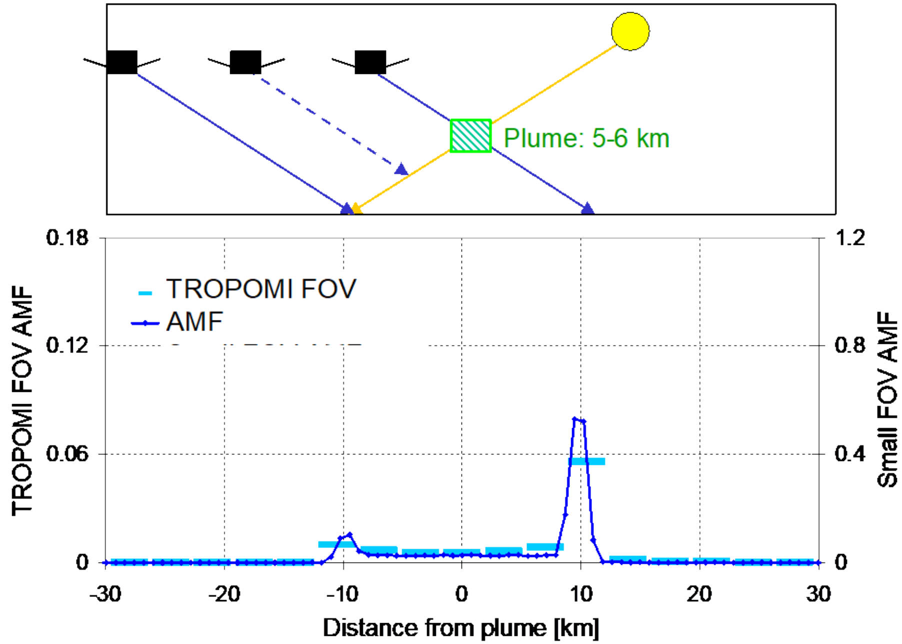
Location of ground pixel(s) ‚seeing the plume' and location of the plume are usually not the same (for elevated plumes)

Geometric effects

c) **VZA: 70, SZA: 0, 5 – 6 km**



d) **VZA: 70, SZA: 60, 5 – 6 km**



Location of ground pixel(s) ‚seeing the plume' and location of the plume are usually not the same (for elevated plumes)

Conclusions

- effect of horizontal light paths can cause systematic and strong underestimation of up to 60% for small FOV like for TROPOMI

- this effect will also be important for other localised plumes, e.g. from power plants, biomass burning, etc.

- the SO_2 saturation effect becomes extremely strong for narrow plumes. The underestimation can become close to 100%; a critical aspect is the switch between different fit windows

- geometric effects become important for high altitude plumes (=> smeared out or double plumes). In extreme cases the ground pixel at the location of the plume will see zero signal.

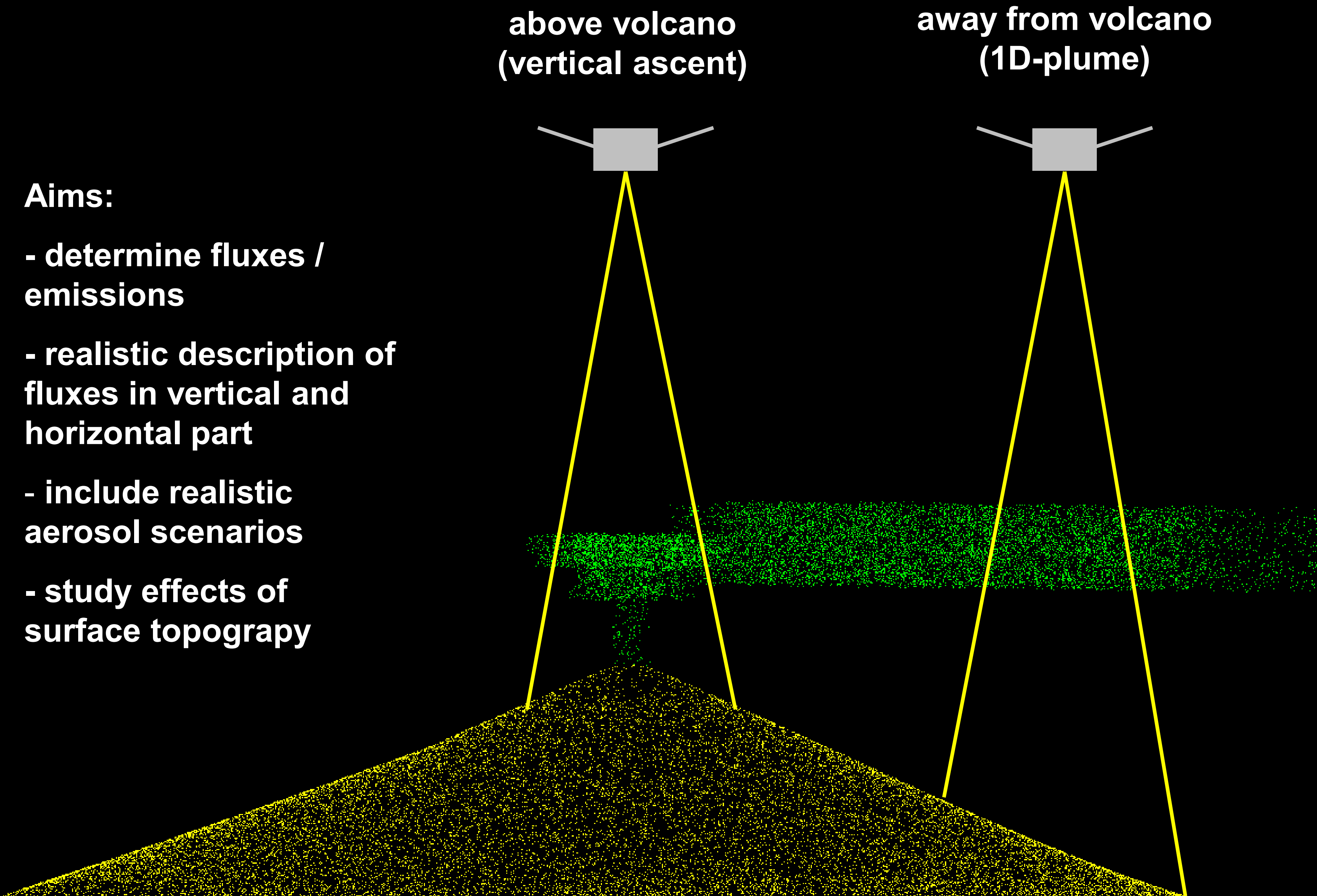
- aerosols modify all three basic 3D effects. They can partly compensate for or increase the underestimation. Side scattering effects can further increase the overestimation for scattering aerosols

- 3D simulations will be applied to ‚realistic‘ volcanic scnearios with focus on localised plumes above the volcano (vertical extended plume) and away from the volcano (horizontal plume).

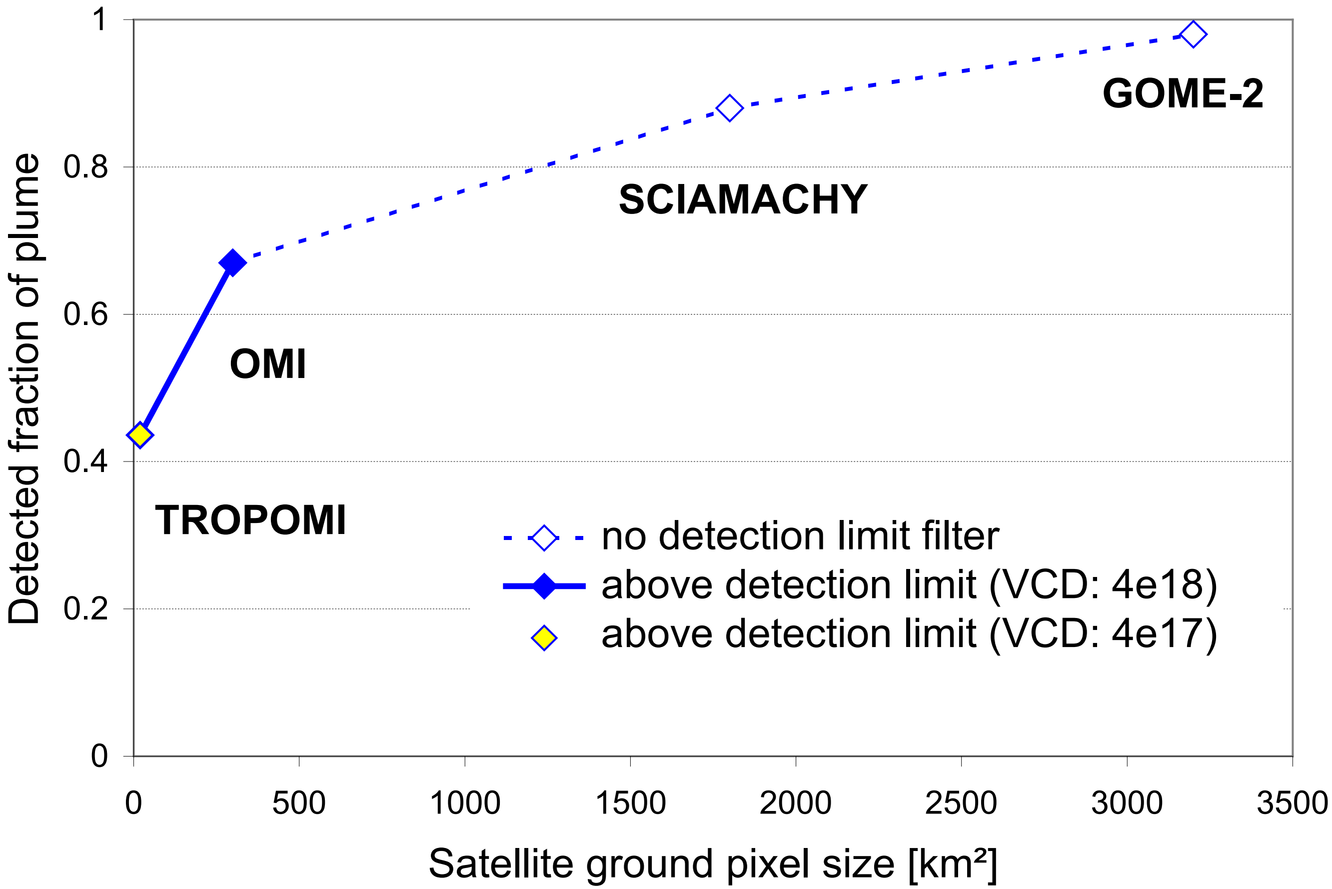
Outlook: simulations for realistic volcanic plumes:

Aims:

- determine fluxes / emissions
- realistic description of fluxes in vertical and horizontal part
- include realistic aerosol scenarios
- study effects of surface topograpy



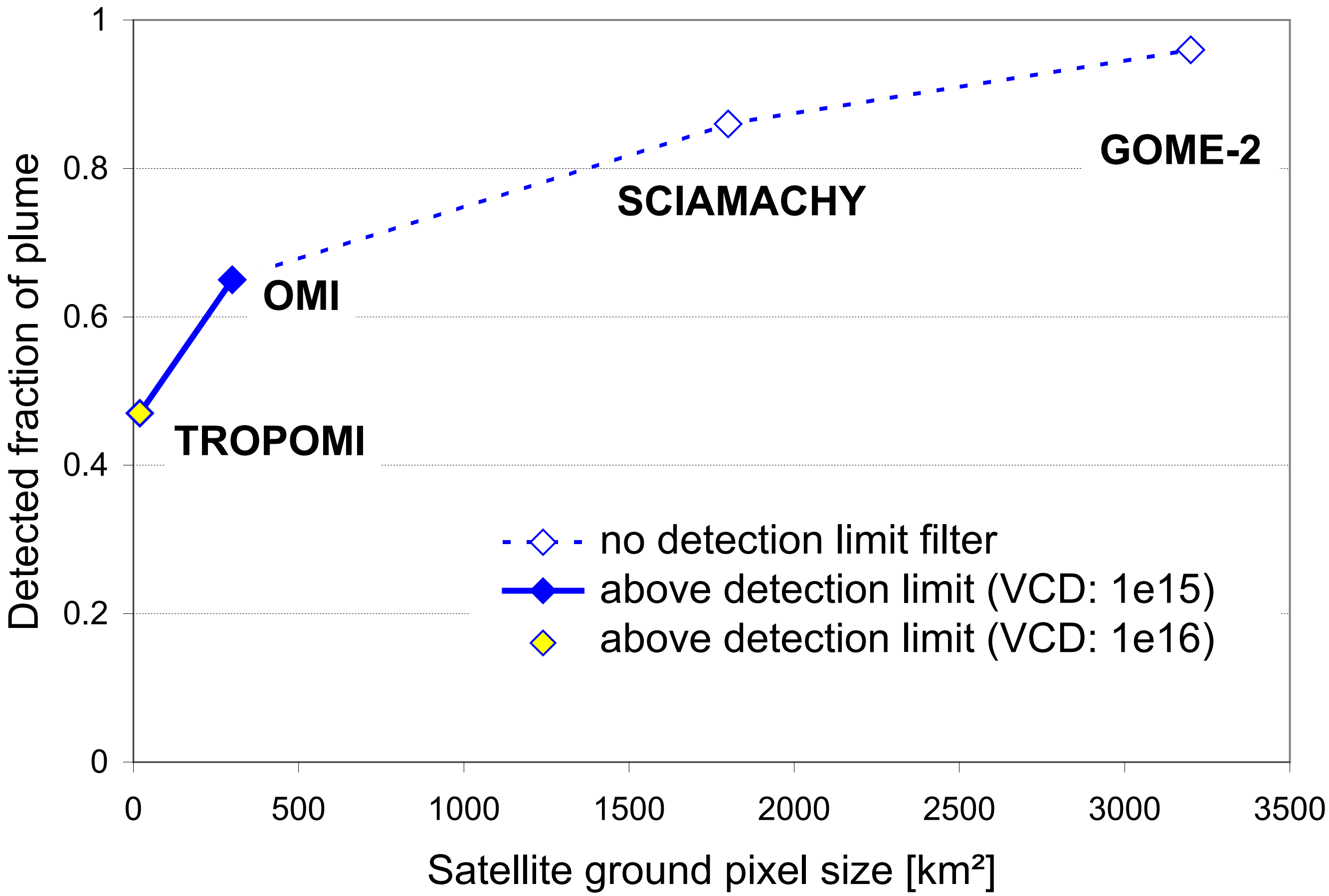
Observations of different instruments of a 1 x 1 x 1 km plume at 5 – 6 km altitude (SO_2 at 313 nm)



The full blue (yellow) symbols indicate observations above the detection limit for a high (low) trace gas VCD

=> narrow plumes can only be observed from instruments with high spatial resolution
=> But for such observations, the adjacency effect is strongest

Observations of different instruments of a 1 x 1 x 1 km plume at 5 – 6 km altitude (BrO at 340 nm)

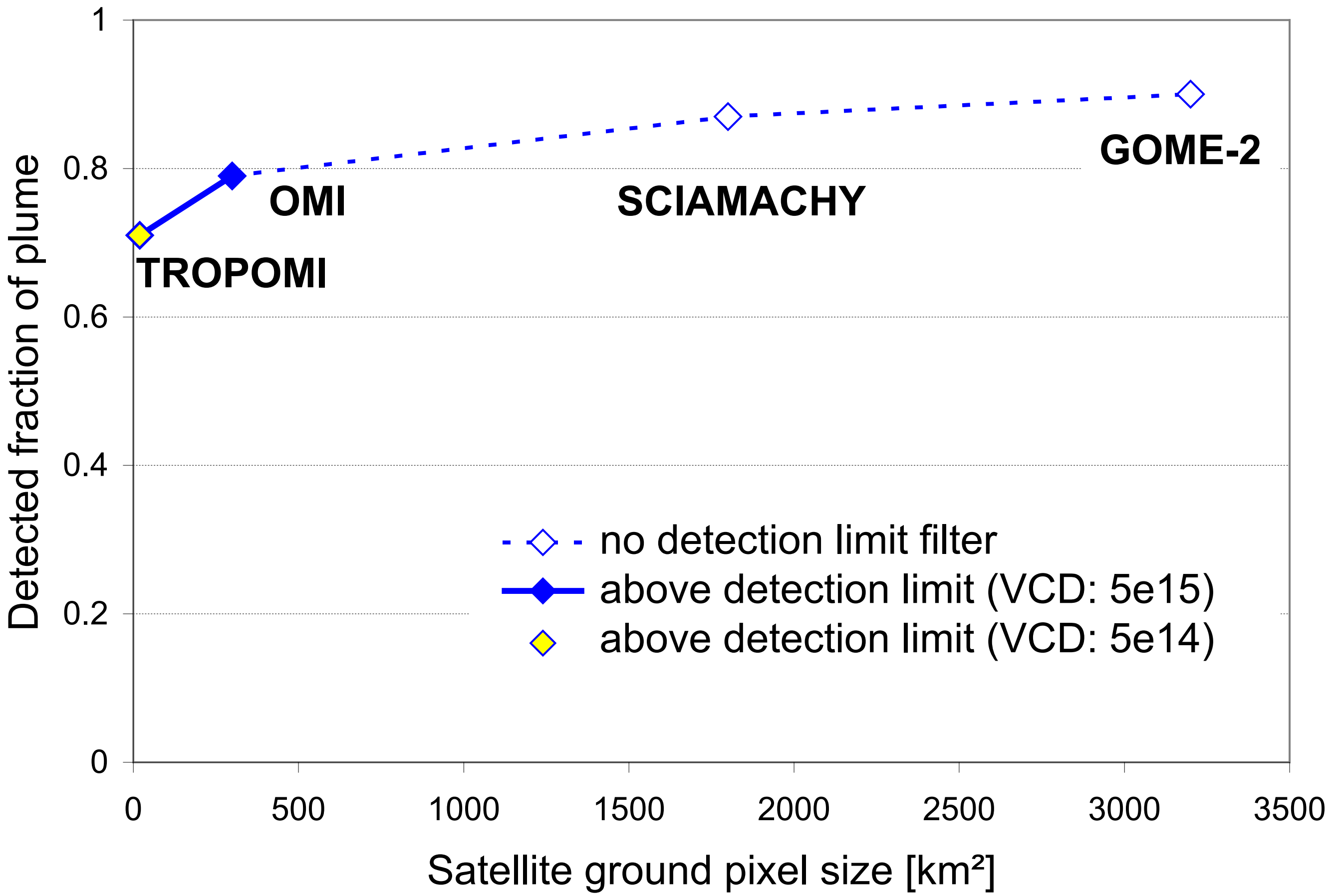


The full blue (yellow) symbols indicate observations above the detection limit for a high (low) trace gas VCD

=> narrow plumes can only be observed from instruments with high spatial resolution

=> But for such observations, the adjacency effect is strongest

Observations of different instruments of a 1 x 1 x 1 km plume at 5 – 6 km altitude (IO at 440 nm)



The full blue (yellow) symbols indicate observations above the detection limit for a high (low) trace gas VCD

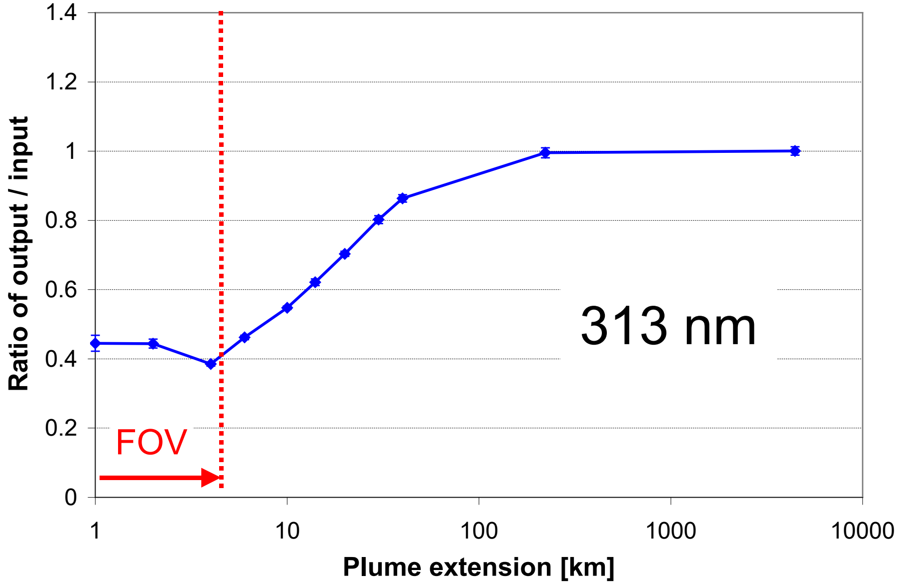
=> narrow plumes can only be observed from instruments with high spatial resolution

=> But for such observations, the adjacency effect is strongest

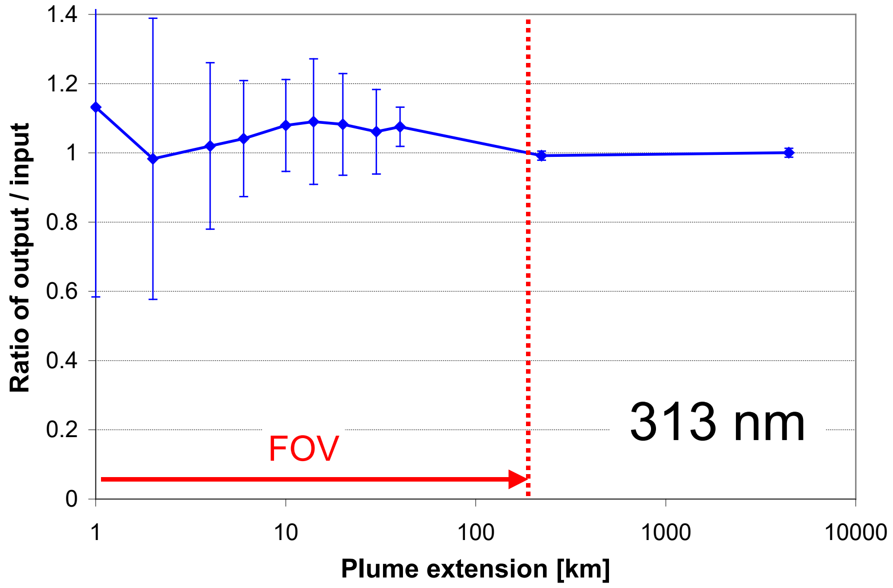
-can increased AMF ‚outside‘ the plume compensate for decrease ‚inside‘ the plume?

The plots show the retrieved fraction of the plume molecules if a 1D-AMF is applied in the analysis

TROPOMI FOV



FOV: 200 x 200km²



=> the underestimation increases towards smaller FOV

=> minimum is found for plume ~ FOV

-if FOV > plume => photons escaping from plume can still be measured

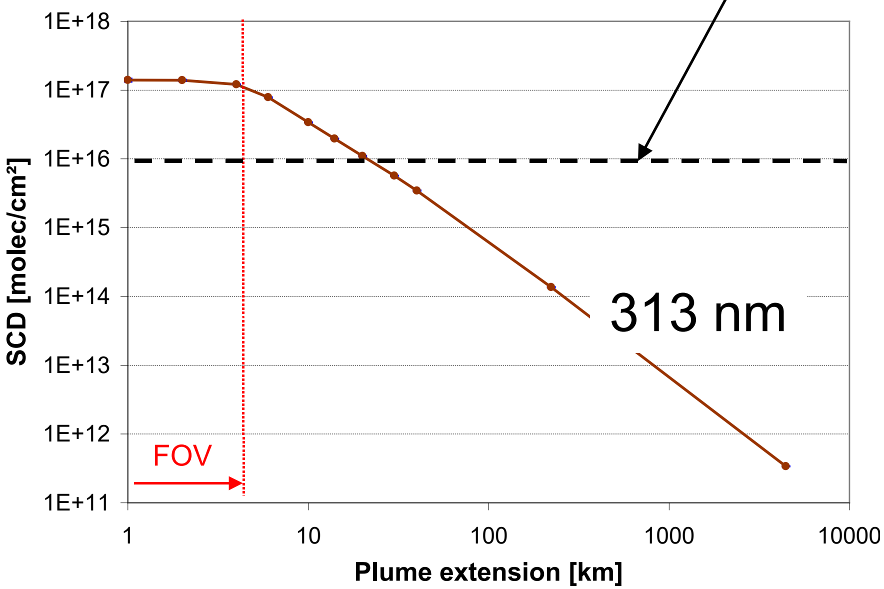
-if plume > FOV => situation becomes similar to 1D case

-can increased AMF ‚outside‘ the plume compensate for decrease ‚inside‘ the plume?

Are the dSCDs still above the detection limit?

TROPOMI FOV

FOV: 200 x 200km²



313 nm

=> Narrow plumes can only be detected by instruments with small ground pixel size