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

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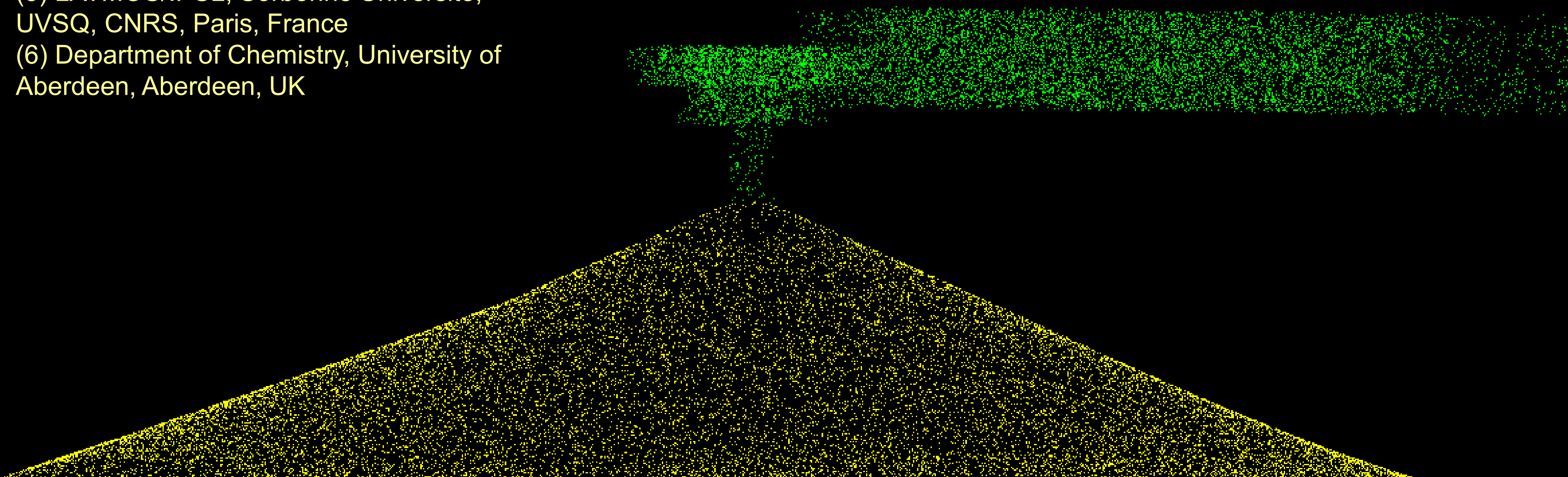
3D RTM simulation of Mt Etna plume with the Monte Carlo Model TRACY-II



Outline:

- motivation
- most important 3D effects:
    - effect of horizontal light paths
    - geometrical effects (SZA, VZA)
    - saturation effects (SO_2)
    - in addition: aerosols effects
- 3D Monte-Carlo RTM simulations (TRACY-2) & model scenarios
- systematic study of the individual effects
- simulations for realistic volcanic plumes

Why are 3D simulations needed?

- pixel size of new satellite sensors is similar to the height of the troposphere and to gradients of atmospheric trace gases and aerosols; also the photon path length in the UV is similar.

  => thus 3D effects become increasingly important

- volcanic plumes show strong spatial gradients with dimensions similar to or smaller than the pixel size of TROPOMI (3.5 x 5.5 km^2)

- so far, horizontally homogenous assumptins (1D-AMFs) are used for analysis of volcanic plumes

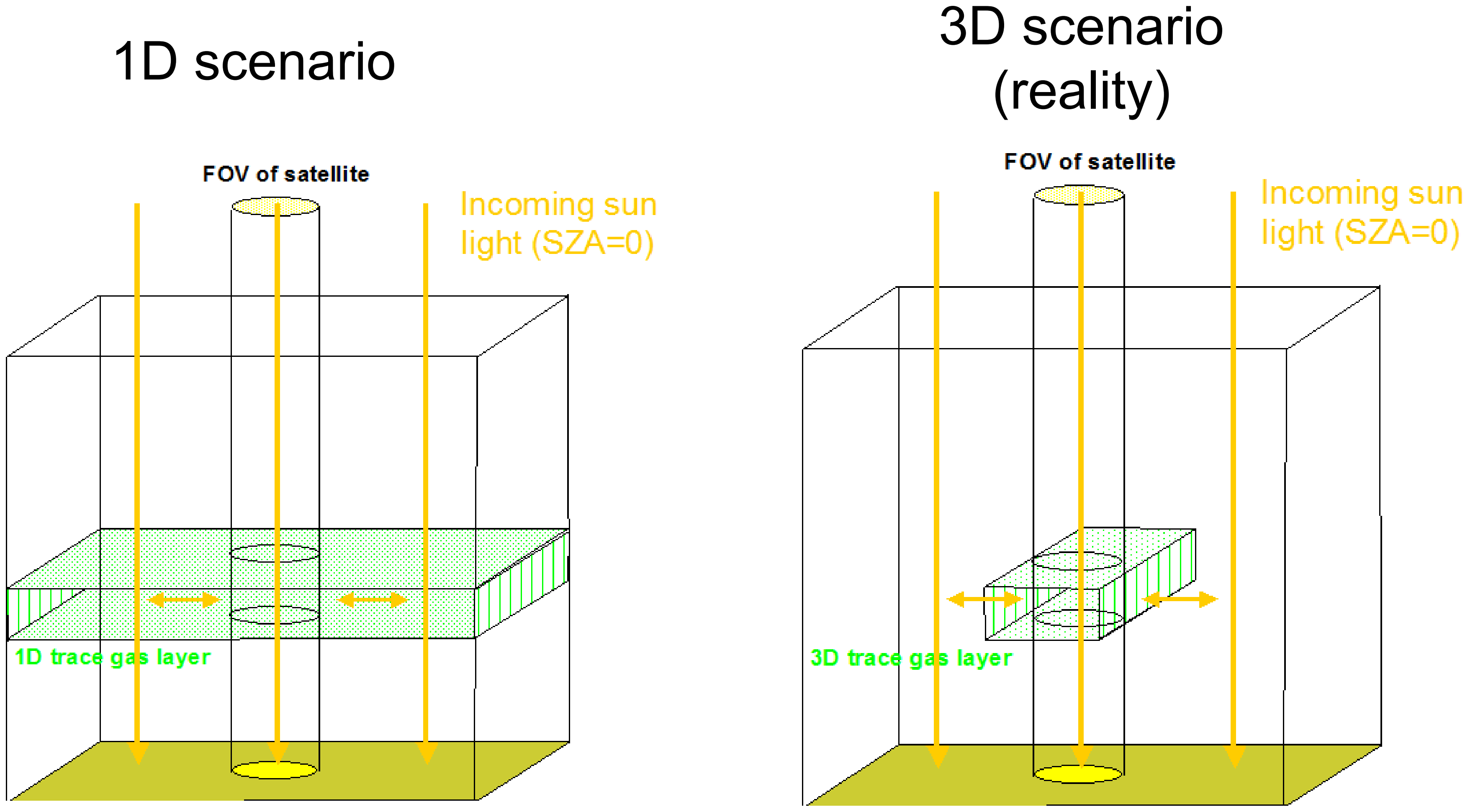
  => how strongly affect 3D effects the satellite results?

- 2 main questions:

  a) how strong does the real (3D) AMF deviate 1D AMF?

  b) what is the effect on the quantitative assessment of volcanic plumes/emissions?

1) Effect of horizontal light paths

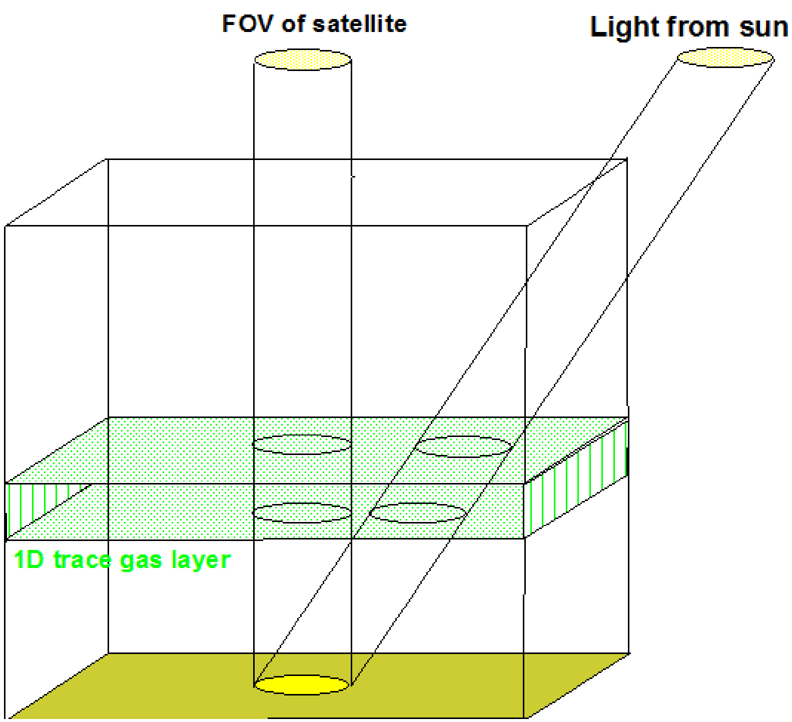


For the 3D case, the photons scattered from outside the plume into the FOV of the satellite don‘t ‚contain‘ a trace gas absorption.

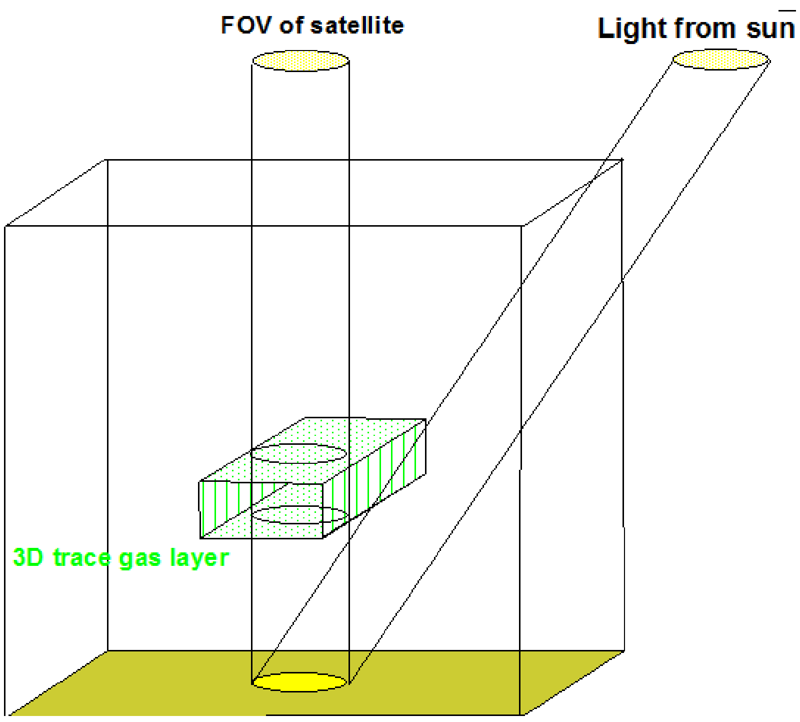
=> the real absorption is lower than the assumed absorption.

2) Geometrical effects (SZA, VZA)

1D scenario



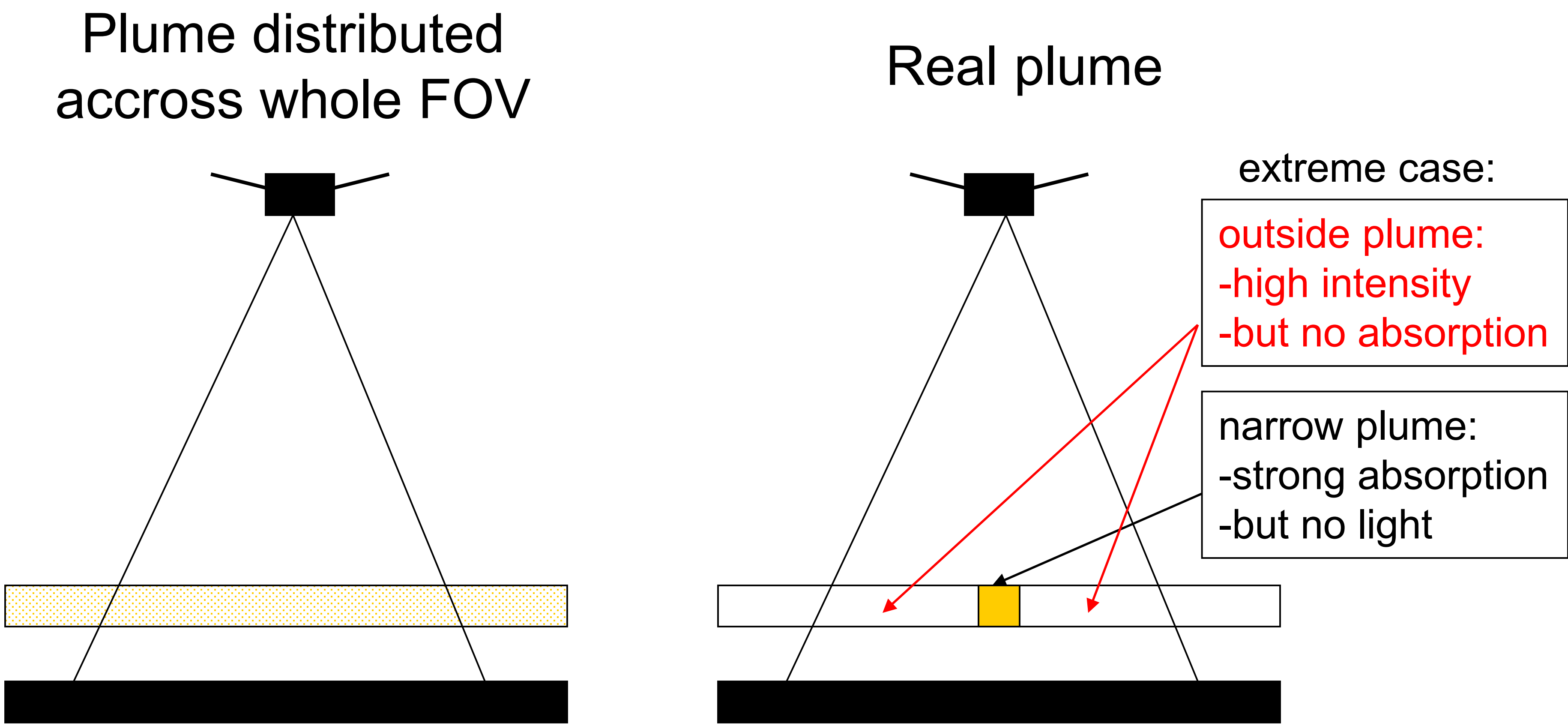
3D scenario (reality)



For the 3D case, the downwards light path might not cross the trace gas layer. (similar effects for changing VZA)

=> the real absorption is lower than the assumed absorption.

3) Saturation effects (for strong SO_2 absorption)



If the plume fills the whole FOV (1D scenario), the true concentration in a narrow plume is strongly underestimated

=> the saturation effect of the real plume is much stronger

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 (1 km – 222 km)
- wavelenths: 315, 350, 440 nm
- FOV: TROPOMI (3.5x5.5km²), 10x10 km²… 200x200 km²

Two comparisons (the two main questions):

a) AMF comparison (plume scans):

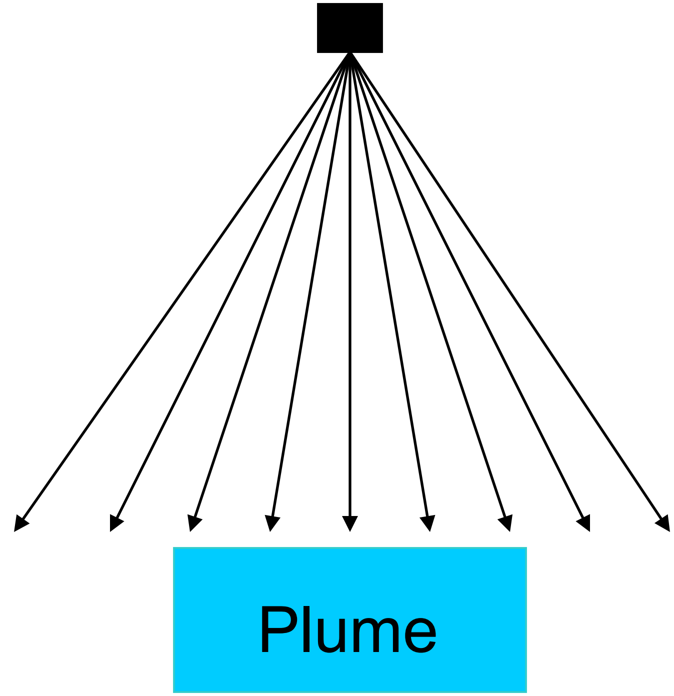
-the AMFs for 3D atmospheres will be compared to the corresponding AMFs for 1D atmospheres

b) output / input comparison (budget plots):

- retrieved number of molcules (with 1D AMF) is compared to the input number of molecules (from 3D simulation)

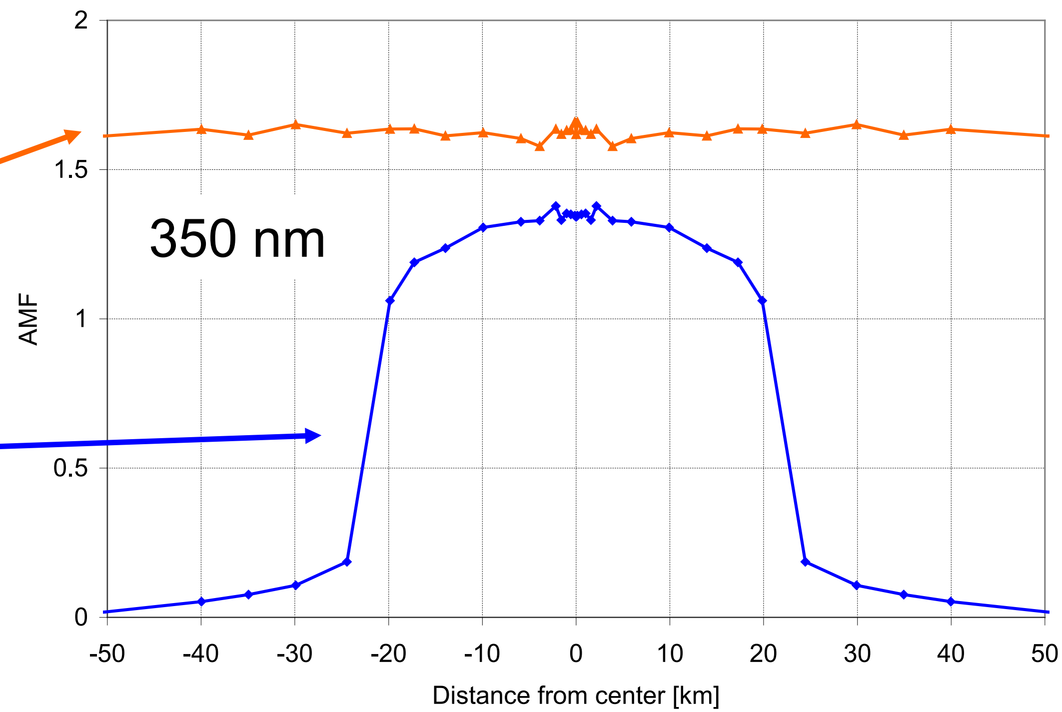
a) Plume scans:
the satellite scans the plume with a narrow FOV

=> information about the spatial variability of the sensitivity to the plume



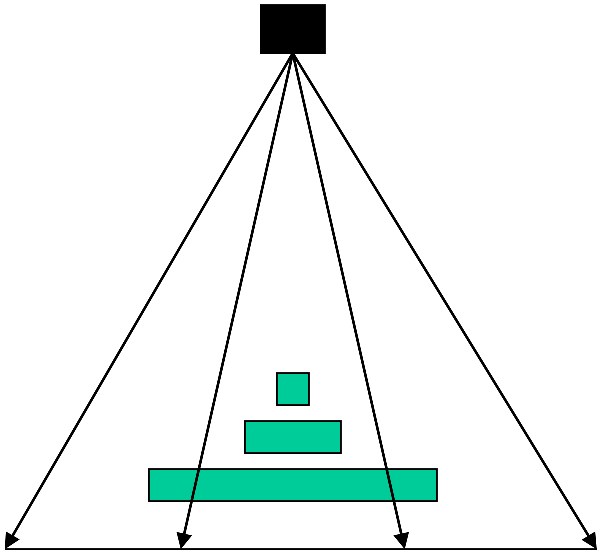
AMF for horizontally extended plume

AMF for 40x 40 km² plume at 5-6 km



b) Budget plots:

Comparison of the retrieved number of molecules to the input number of molecules for different plume sizes and FOV

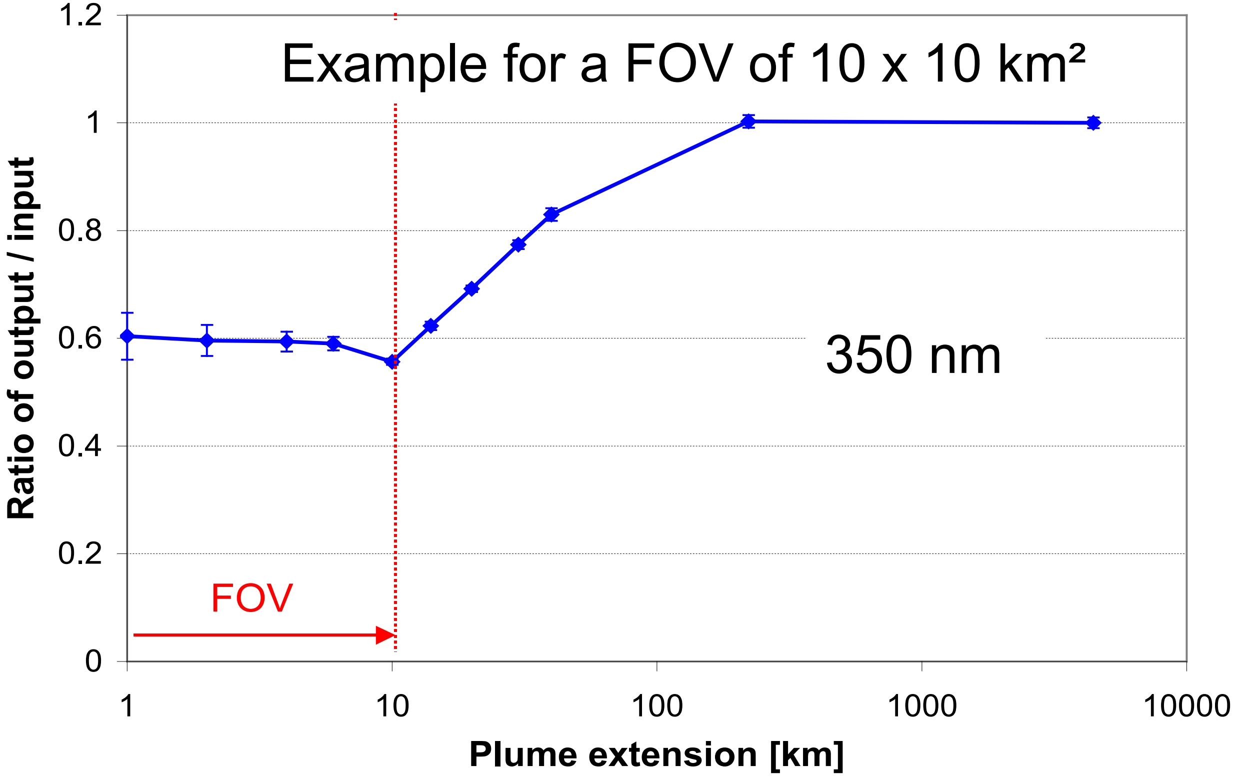


calculation of the number of molecules:

-the derived SCD for a given FOV is divided by the coresponding **1D AMF**

=> ‚effective‘ VCD for FOV

-the effective VCD is multiplied by the area of the FOV



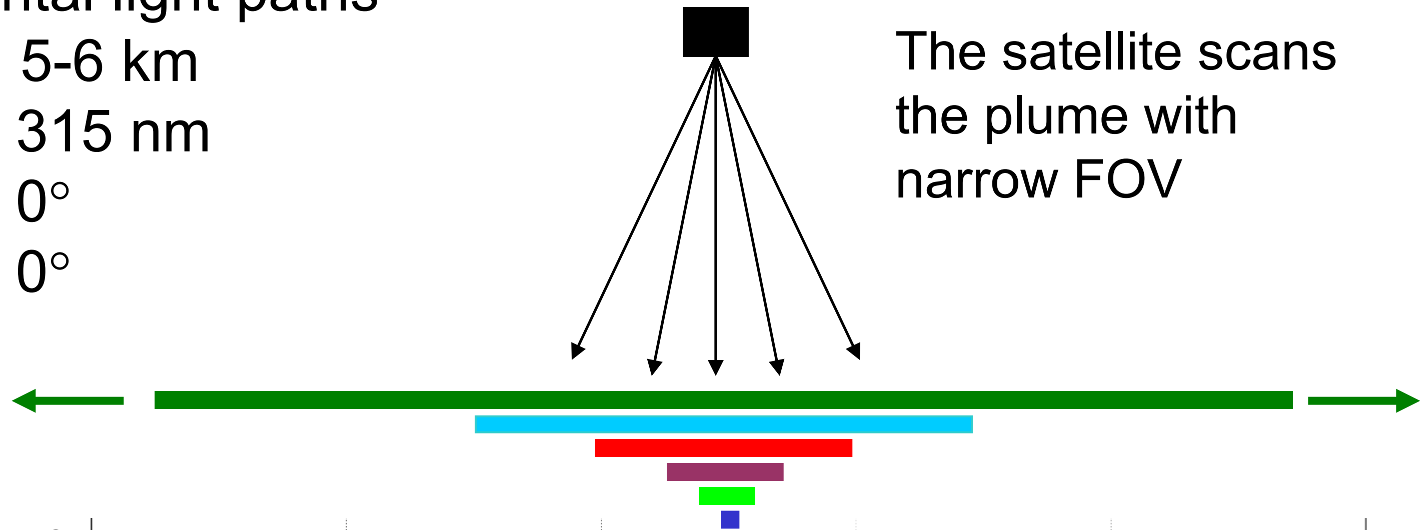
Effect 1: Horizontal light paths

Plume altitude: 5-6 km

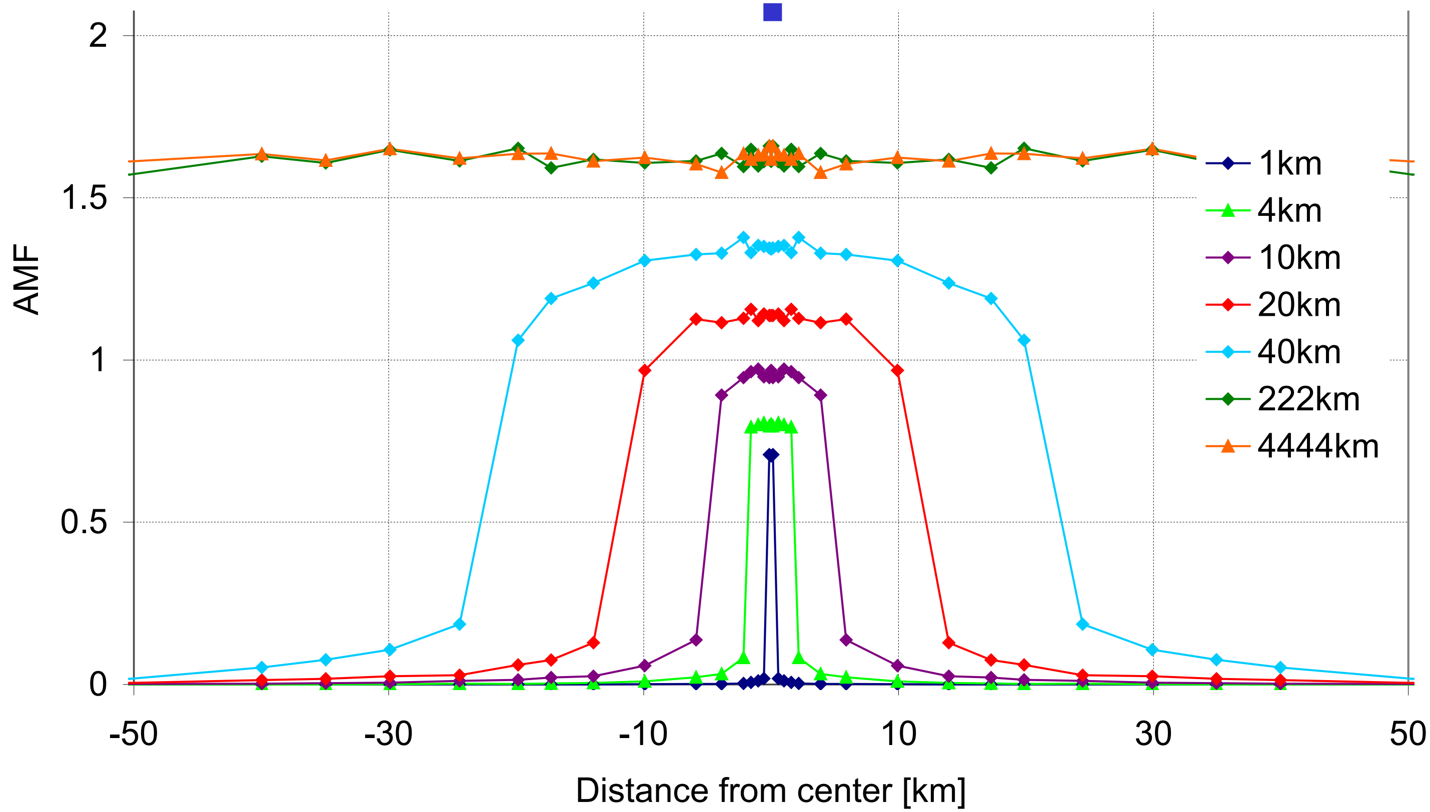
Wavelength: 315 nm

SZA: 0°

VZA: 0°



The satellite scans the plume with narrow FOV

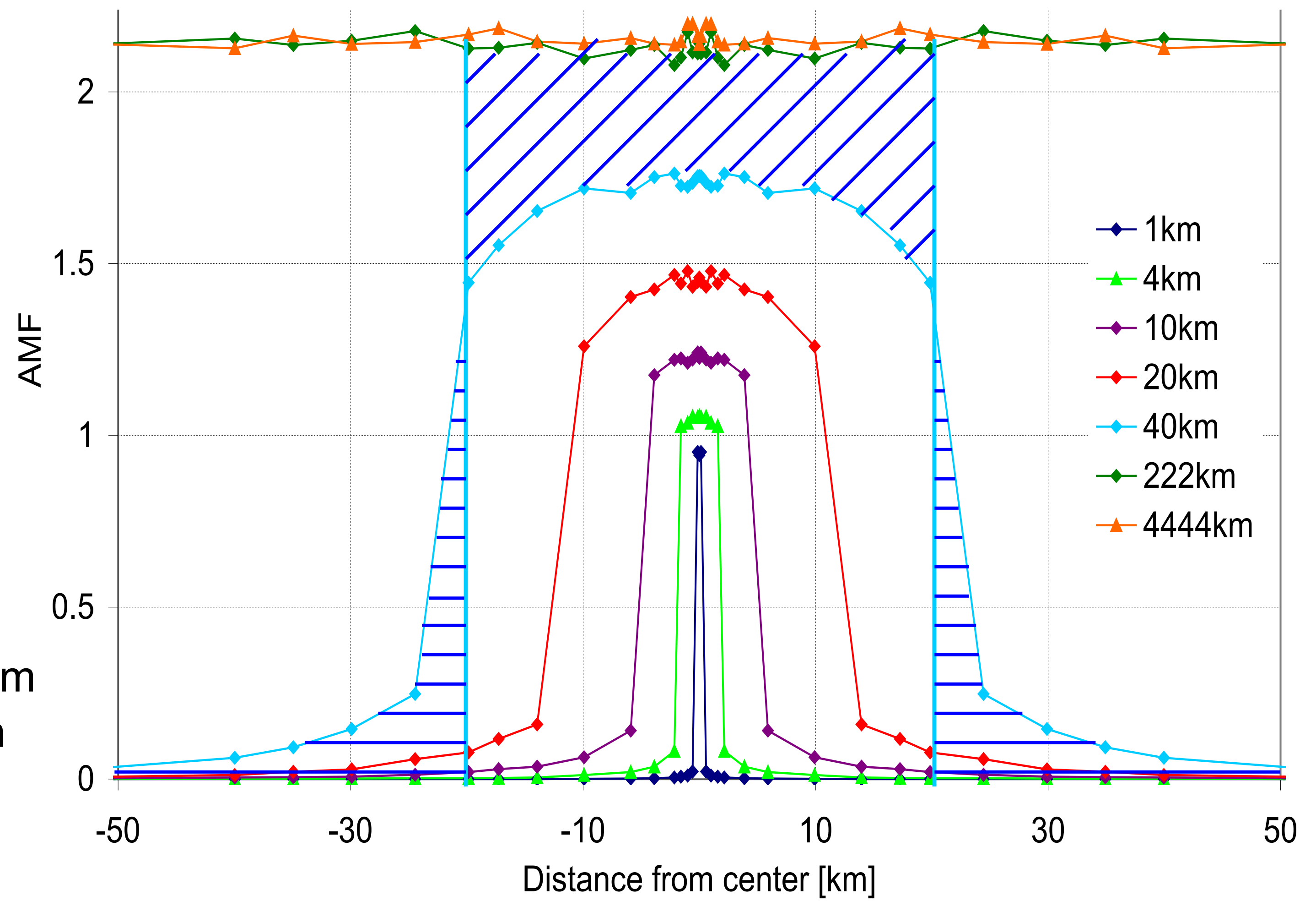


=> for narrow plumes the AMFs are strongly reduced

=> there are no sharp edges

Effect 1: Horizontal light paths

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

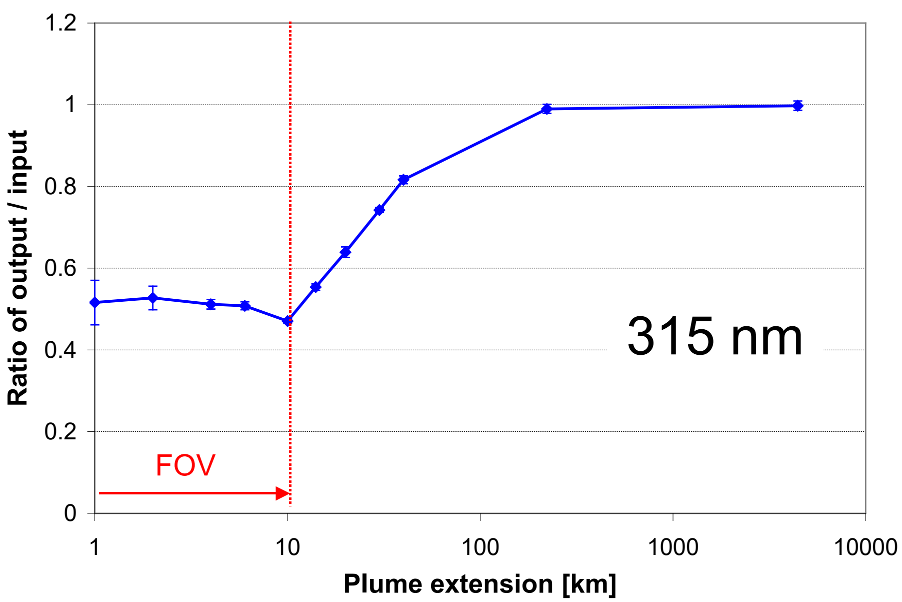


altitude: 10-11 km
Wavelength: 315 nm
SZA: 0°
VZA: 0°

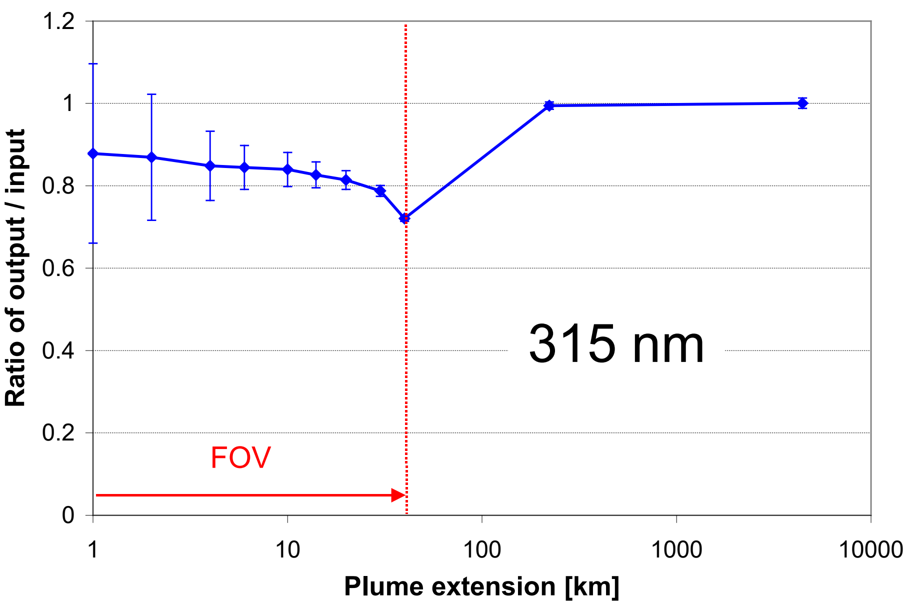
Effect 1: Horizontal light paths

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

FOV: 10 x 10km²



FOV: 40 x 40km²



=> the underestimation increases towards smaller FOV

=> minimum is found for plume = FOV

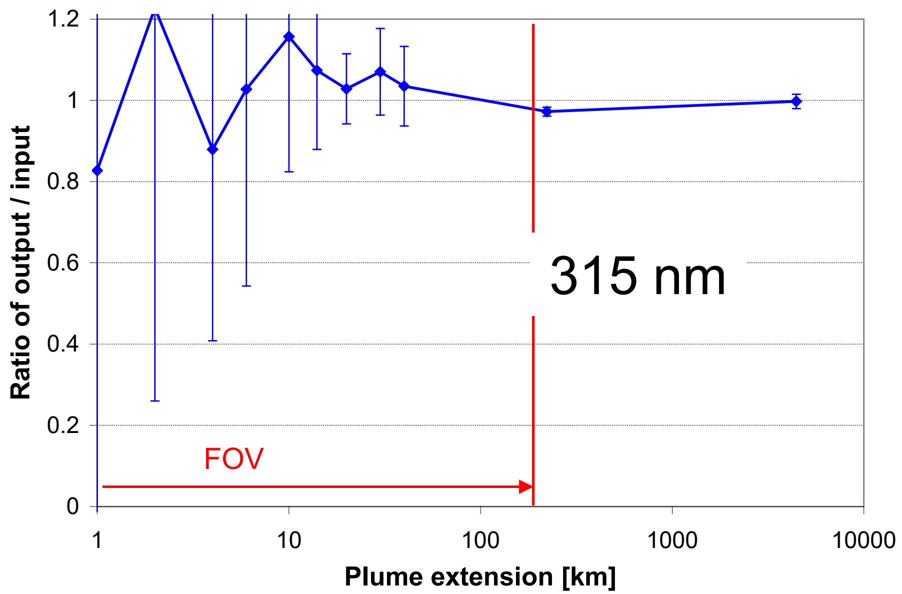
-if FOV > plume => photons escaping from plume can still be measured

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

Effect 1: Horizontal light paths

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

FOV: 200 x 200km²



These results are for a plume altitude of 5-6 km; similar results are obtained for other wavelengths and altitudes

=> For plume >> FOV, all molecules are measured, even using the 1D AMF

(very large scatter for small plumes, because they fill only very small fraction of FOV: for 1km² plume the fraction is 0.000025)

Effect 1: Horizontal light paths

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

0.25%	0.5%	0.6%	0.5%	0.25%
0.5%	2%	4.7%	2%	0.5%
0.6%	4.7%	65%	4.7%	0.6%
0.5%	2%	4.7%	2%	0.5%
0.25%	0.5%	0.6%	0.5%	0.25%

=> Total 99.2%

FOV 20x20 km^2

Plume 10x10 km^2

Effect 1: Horizontal light paths

-What about the absorption strength?

assume a BrO VCD of 1e14 molec/cm^2 in the plume.

BrO optical depth at 350 nm

<1e-5	<1e-5	<1e-5	<1e-5	<1e-5
<1e-5	<1e-4	<1e-4	<1e-4	<1e-5
<1e-5	<1e-4	7.7e-4	<1e-4	<1e-5
<1e-5	<1e-4	<1e-4	<1e-4	<1e-5
<1e-5	<1e-5	<1e-5	<1e-5	<1e-5

FOV 20x20km^2

Plume 10x10km^2

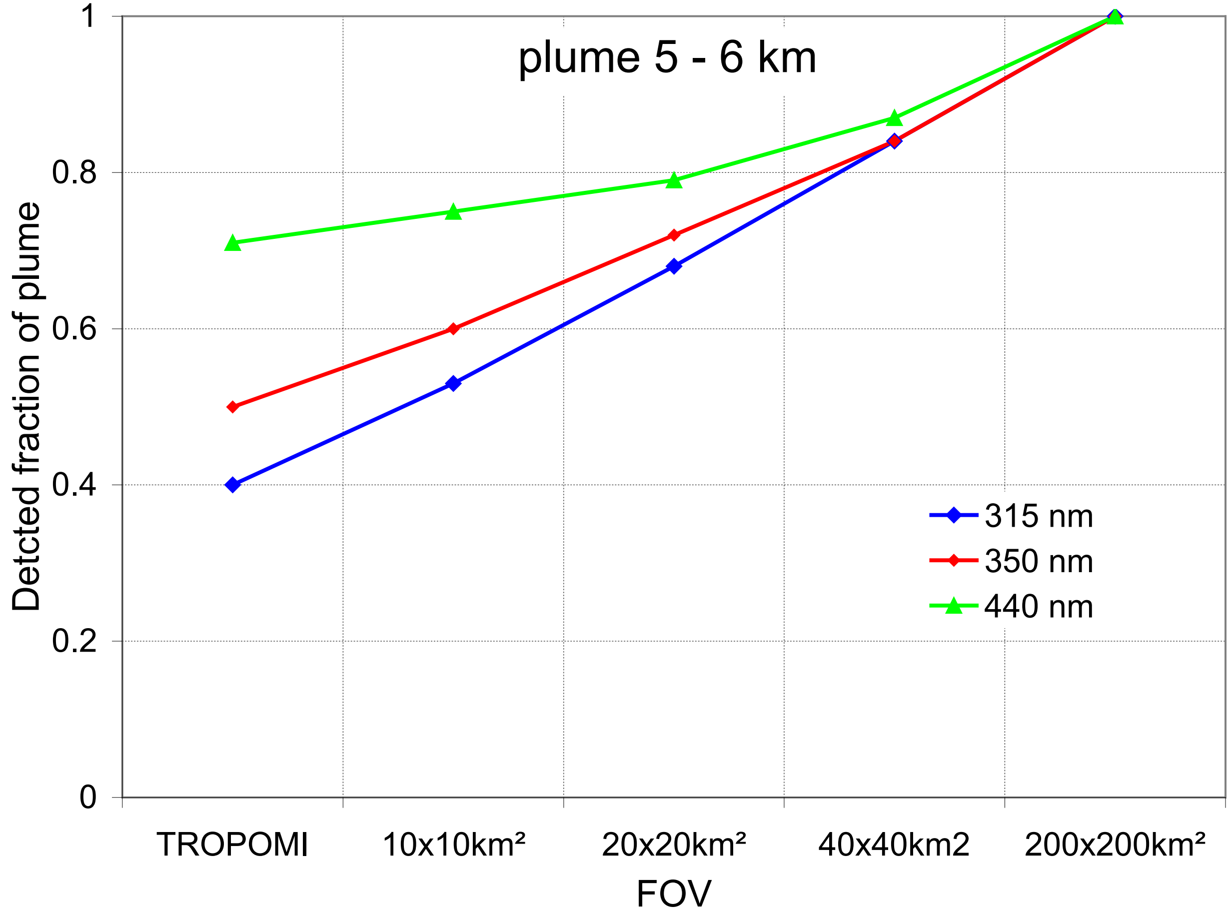
the signal for all pixels outside the center pixel is below the detection limit.

=> only ~ 68% of the plume will be detected

Effect 1: Horizontal light paths

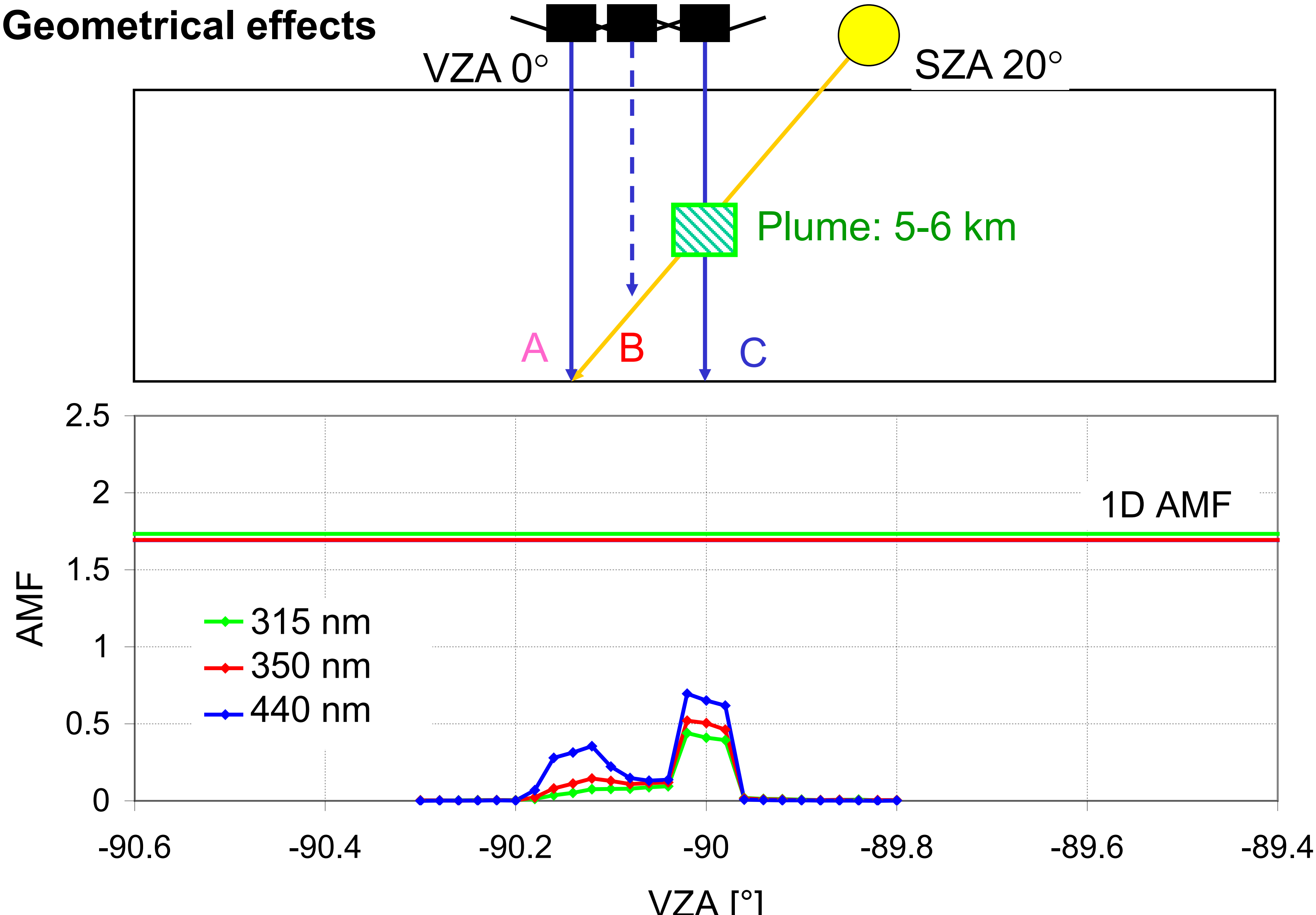
Fraction of detected plume molecules as function of the FOV for different wavelengths

Plume area: 2 x 2 km²



Similar results for other plume altitudes

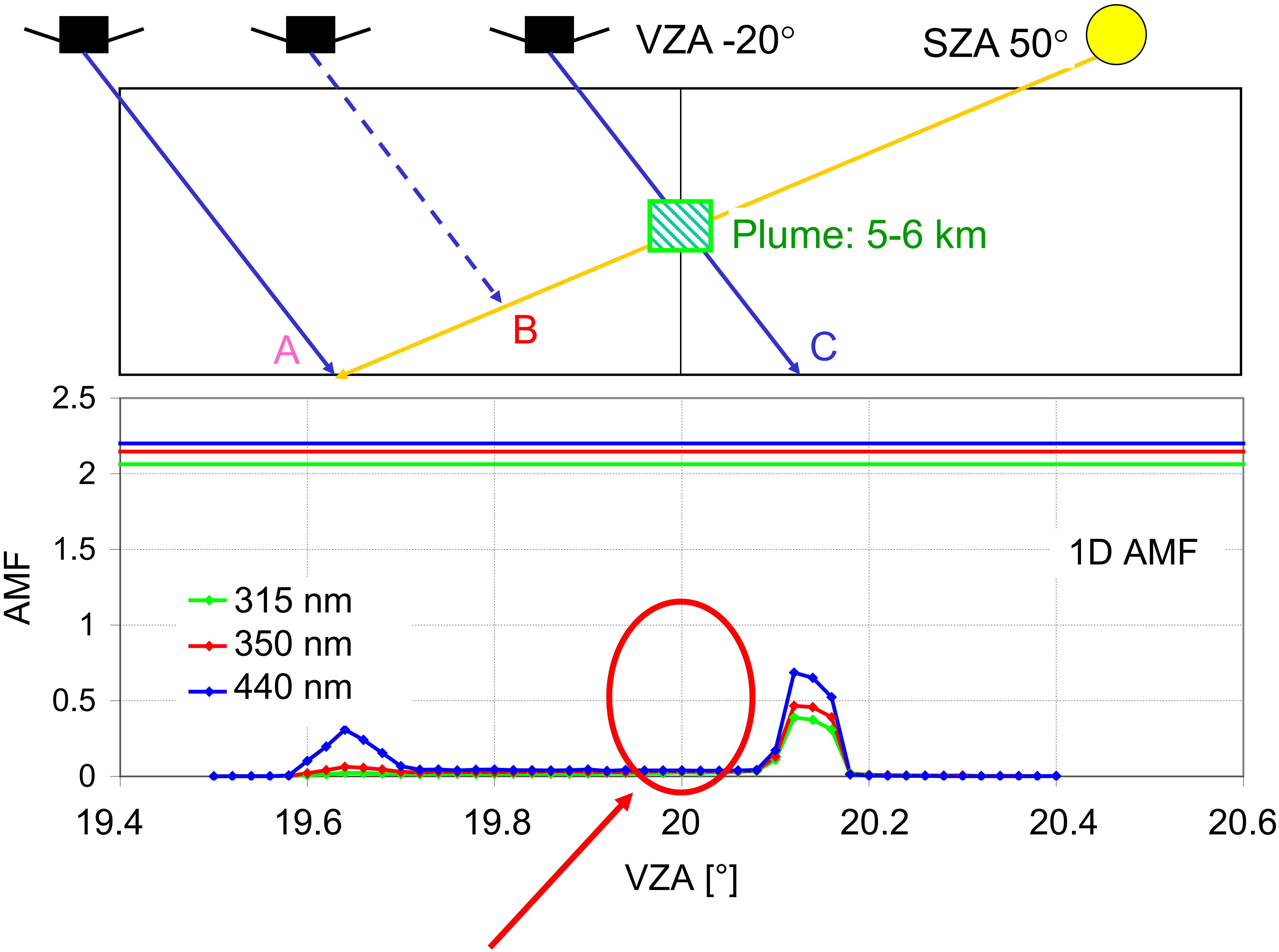
2) Geometrical effects



A: direct sun light crosses plume and is reflect at surface

B: direct sun light crosses plume and is scattered

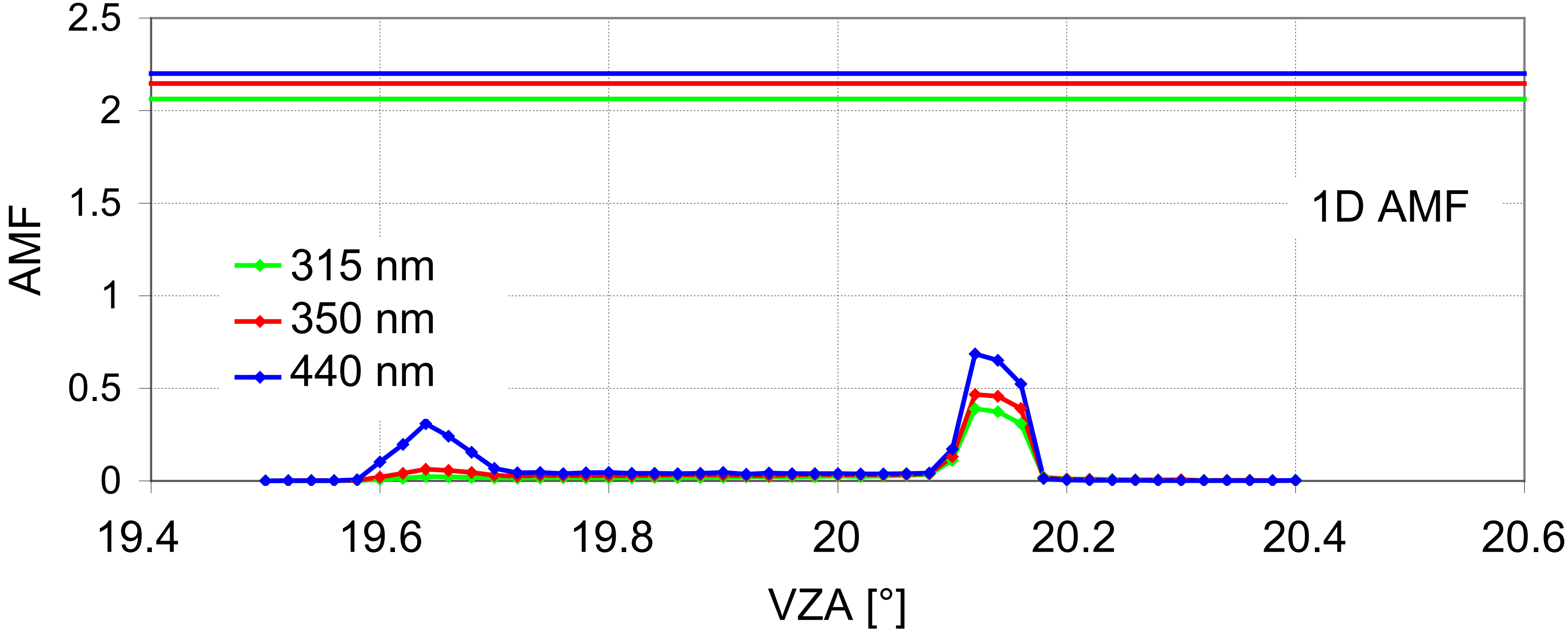
C: line of sight crosses plume



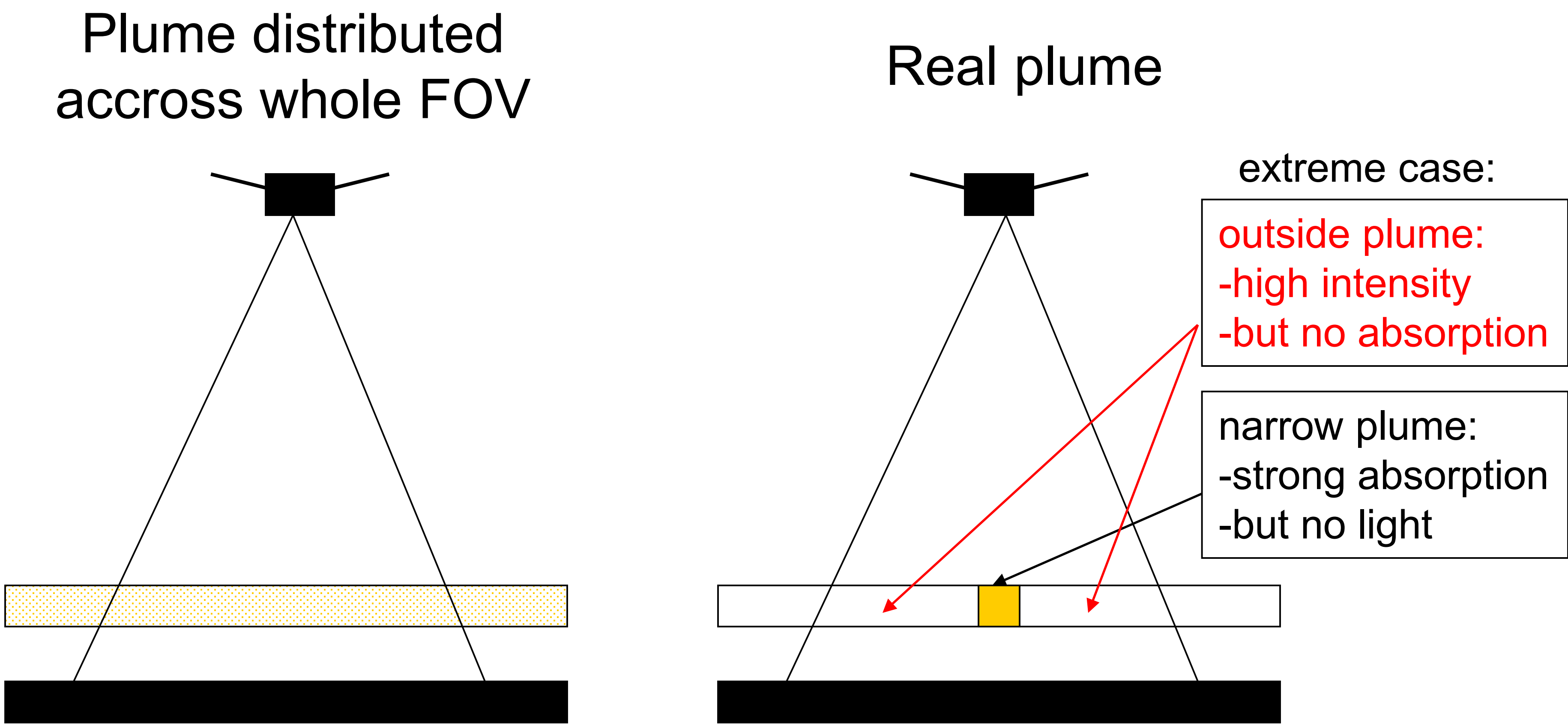
In extreme cases the plume is not seen at the location where it is

2) Geometrical effects

-effect of horizontal light paths still is similar as shown before
-for plumes at high altitudes, multiple plumes might be ‚seen' by the satellites



3) Saturation effects (for strong SO_2 absorption)



If the same amount of molecules is contained in both plumes, the concentration in the 1D scenario is much lower than in reality.

=> the saturation effect of the real plume is much stronger

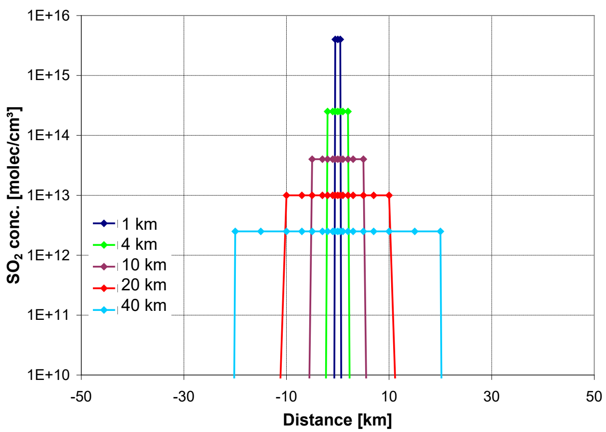
3) Saturation effects (for strong SO_2 absorption)

the maximum VCDs for narrow plumes are taken from literature, e.g. 2.4e20 molec/cm² (Kern et al., 2020).

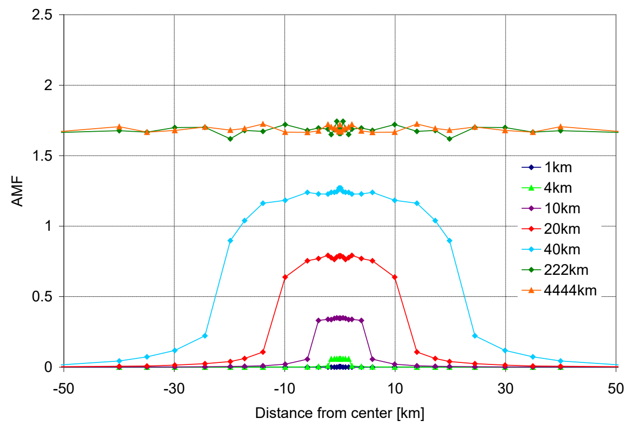
For a 1x1x1km³ plume this equals 2.4e30 molecules

simulations for 310 nm

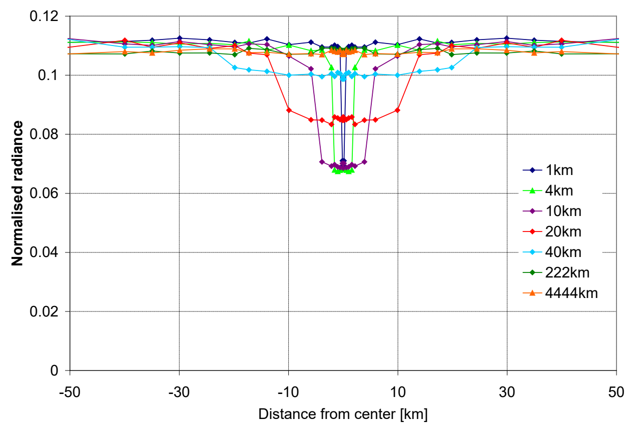
plume concentrations



AMF for plume scans



radiances for plume scans



(maximum VCD: 4e20)

-very low AMF for high concentrations

-very low radiances for high concentrations

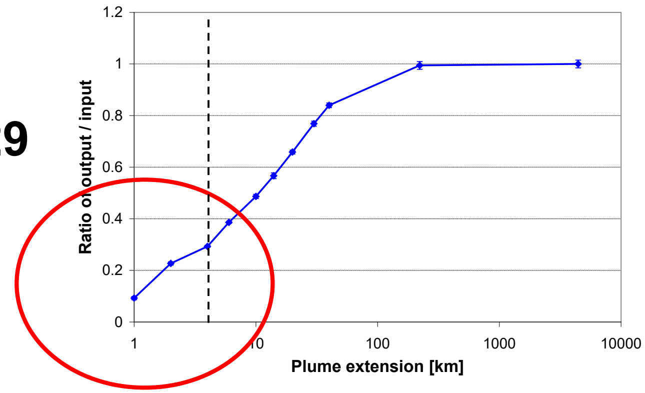
3) Saturation effects (for strong SO_2 absorption)

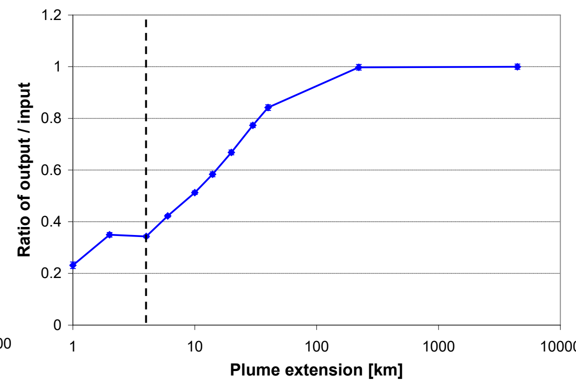
FOV: TROPOMI

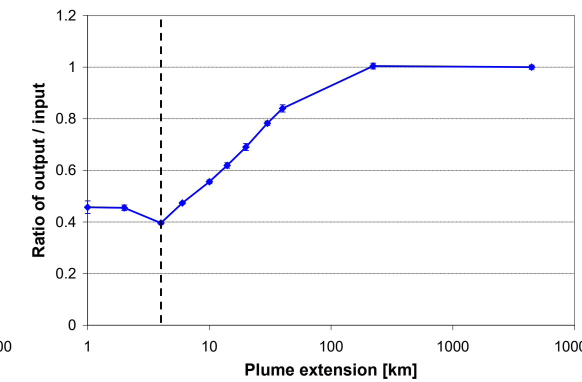
number of molecules

310 nm | **317 nm** | **332 nm**

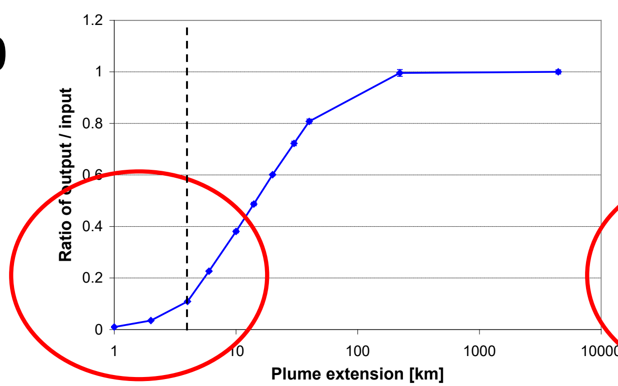
1e29

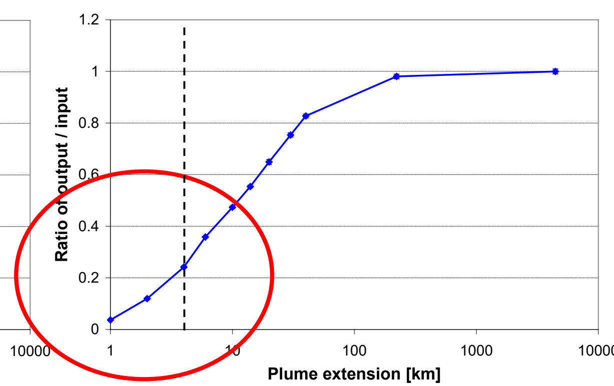


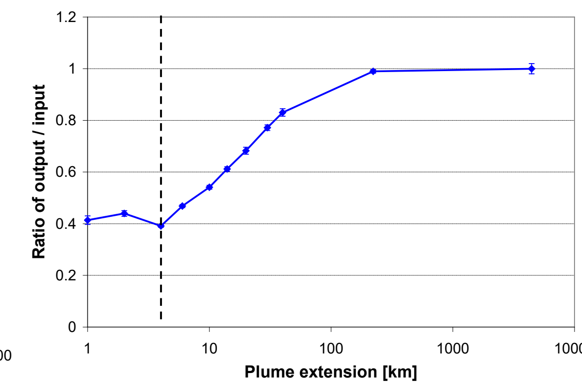




1e30







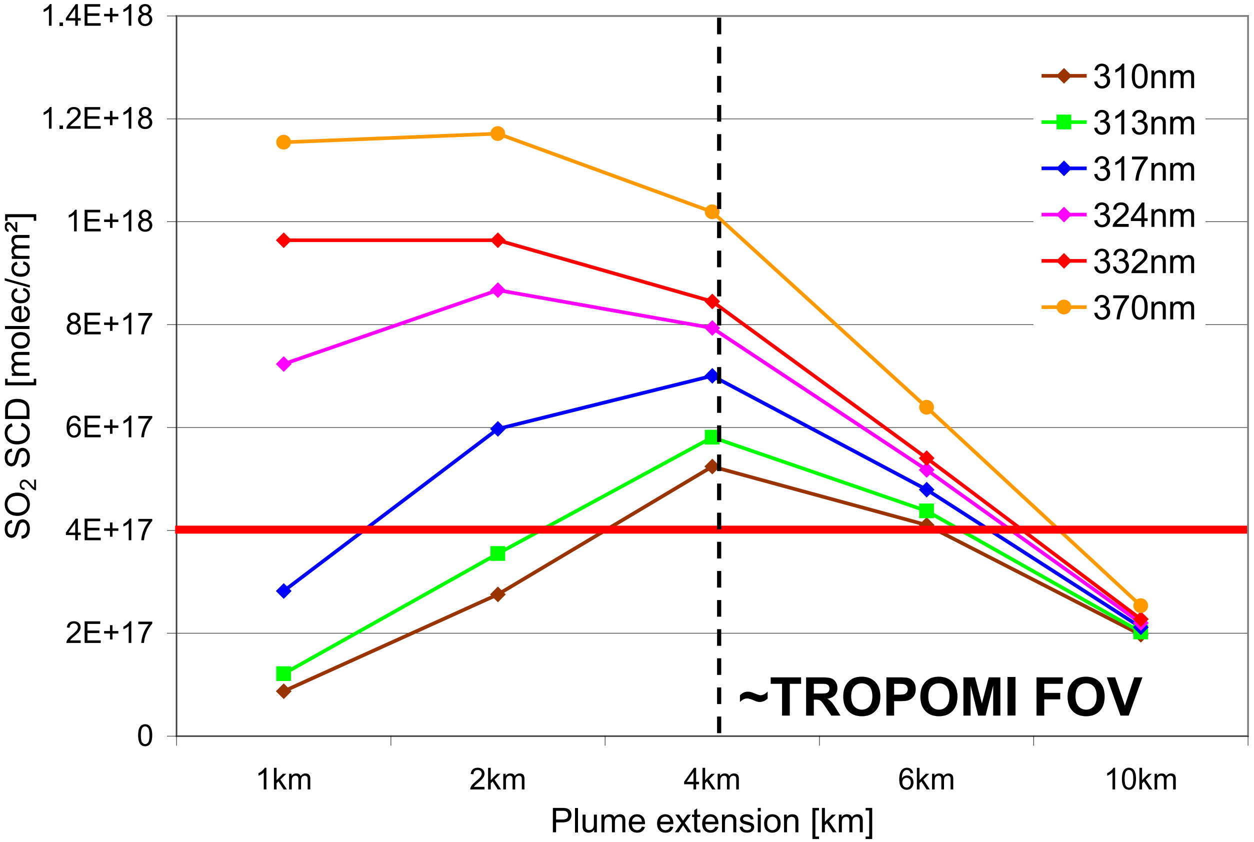
=> very low effective AMFs for narrow plumes

=> underestimation depends on the SO_2 amount and wavelength

3) Saturation effects (for strong SO_2 absorption)

Max. plume concentration
[molec/cm³]

The same number of molecules ($2.5*10^{29}$) is contained in plumes of different horizontal extension



Threshold to switch fit window for TROPOMI SO_2 analysis

=> always look at results from different wavelength ranges!

For a narrow plume, very low SCDs are measured

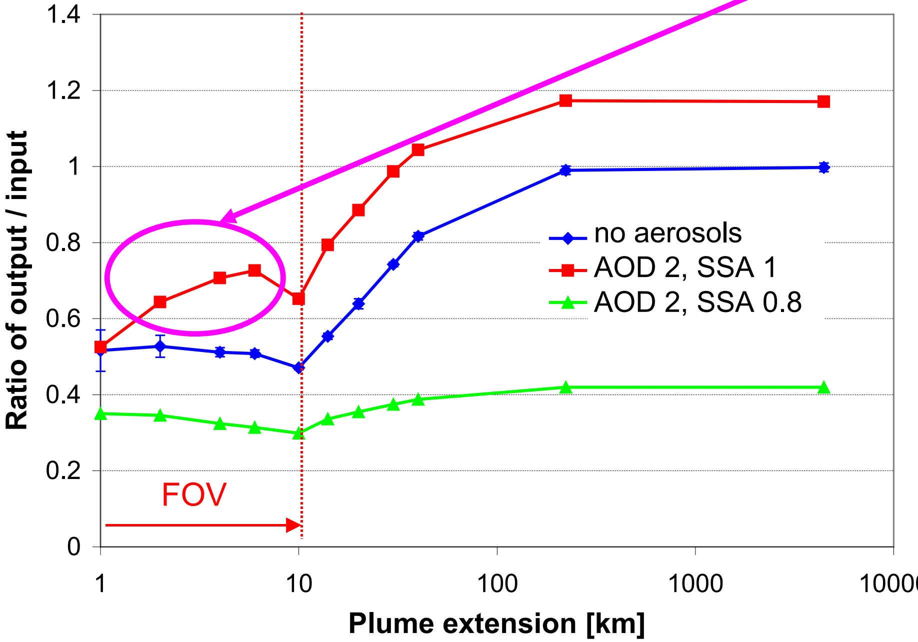
Effects of aerosols

-aerosol influence all 3D effects discussed before
-here we only show the effects related to horizontal light paths
-general assumption: aerosols and trace gases are in the same volume
-the other effects will be studied in the near future

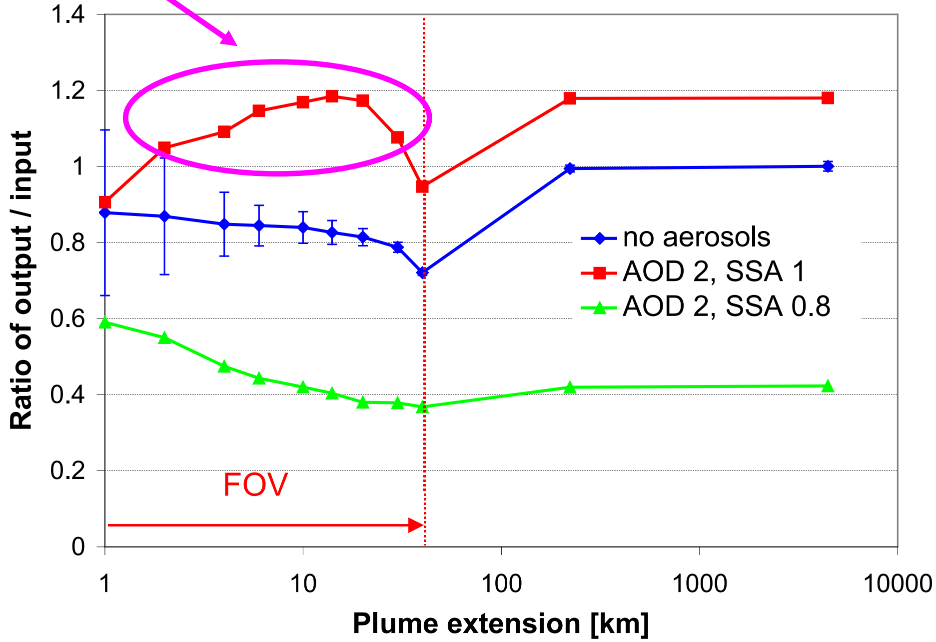
Results for 315 nm and plume at 5-6 km

effect of enhanced multiple scattering

FOV: 10 x 10 km²



FOV: 40 x 40 km²

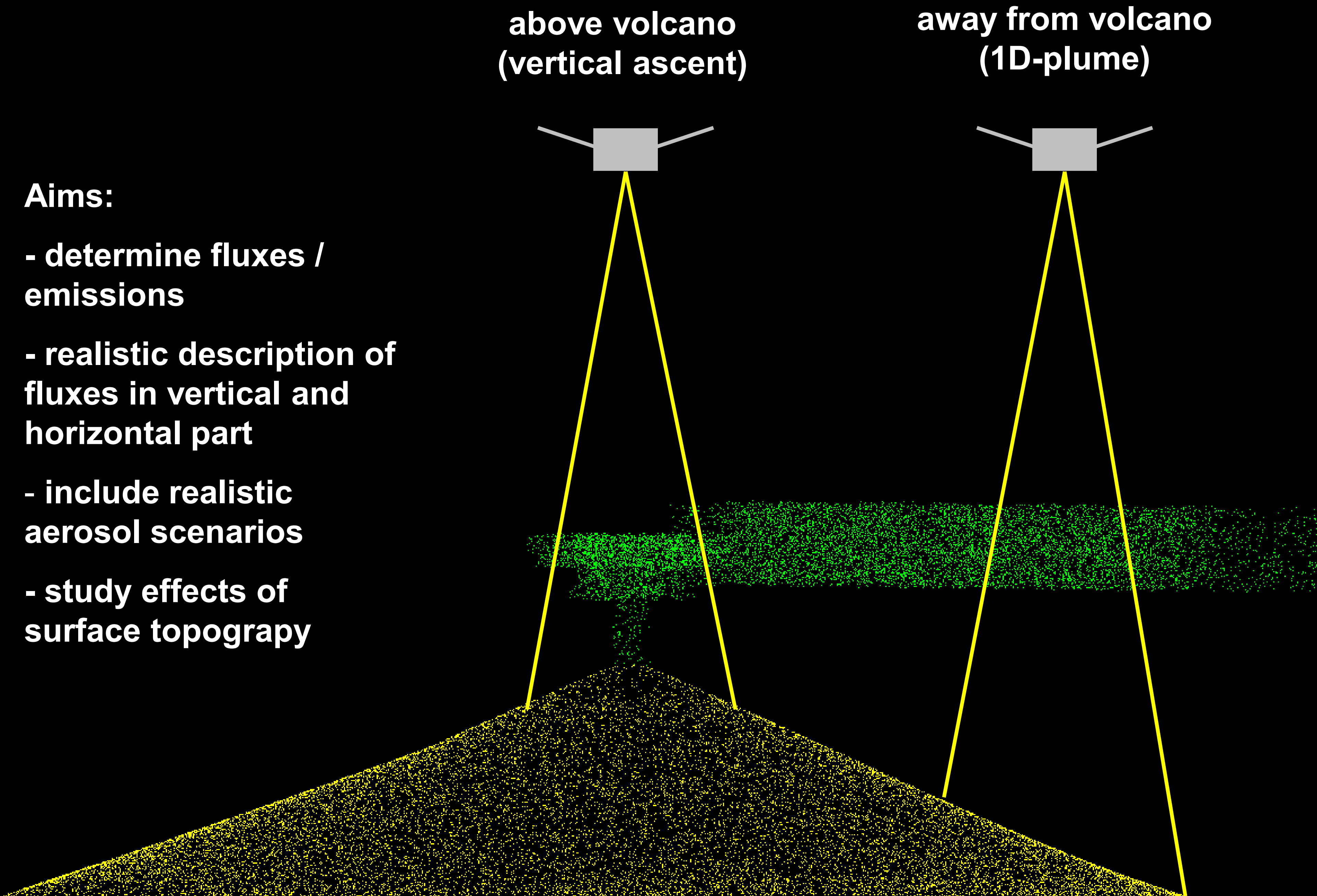


=> aerosols can enhance or decrease the sensitivity

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



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.

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

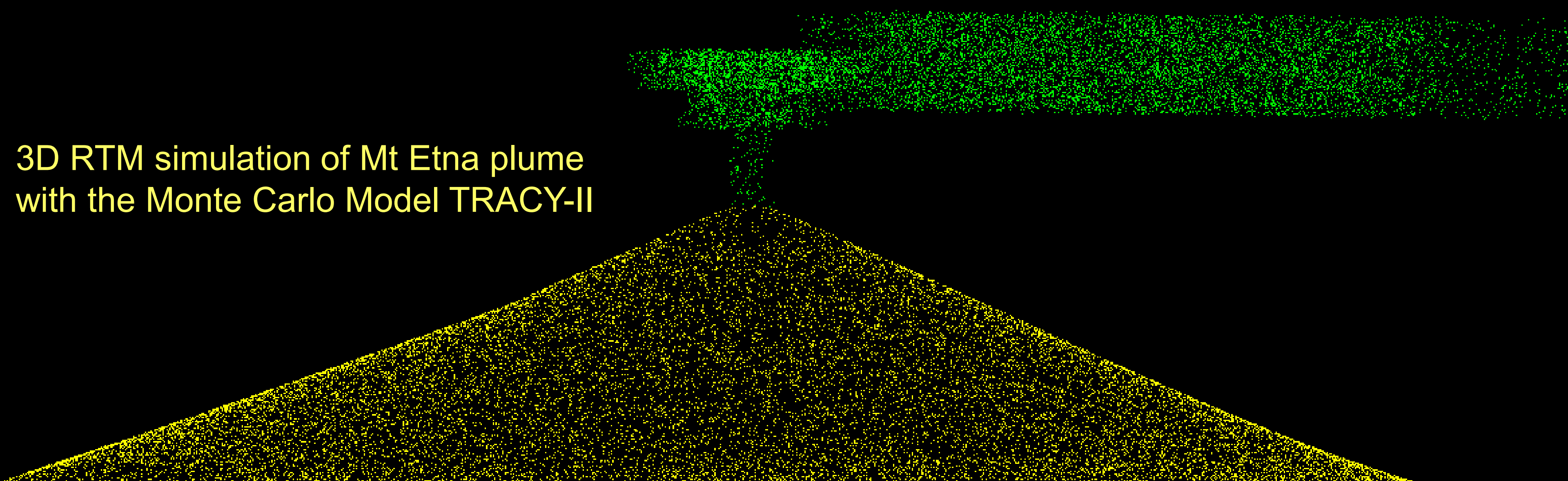
- the SO_2 saturation effect becomes extremely strong for narrow plumes. The underestimation can become close to 100%; a critical aspect is that the switch between different fit windows can be strongly affected.

- aerosols modify all three basic 3D effects. They can partly compensate for or increase the underestimation; further investigation is needed.

- 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).

- similar investigations will be performed for ground based measurements.

Many thanks for your attention



3D RTM simulation of Mt Etna plume
with the Monte Carlo Model TRACY-II

3) Saturation effects (for strong SO_2 absorption)

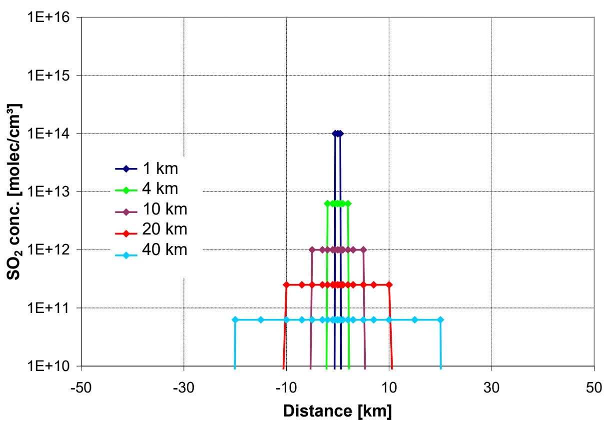
-simulations for SO_2 plumes of different horizontal extensions are performed

-all plumes contain the same number of molecules; thus the concentration and the VCD depend on the horizontal plume extension

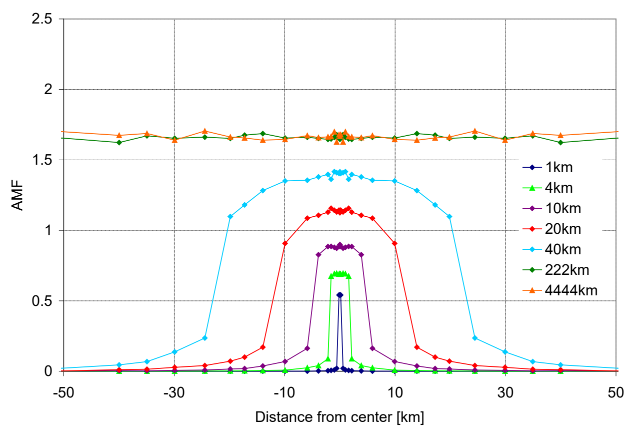
-the maximum VCDs are taken from published values, e.g. 2.4e20 molec/cm² as in Kern et al., 2020

simulations for 332 nm

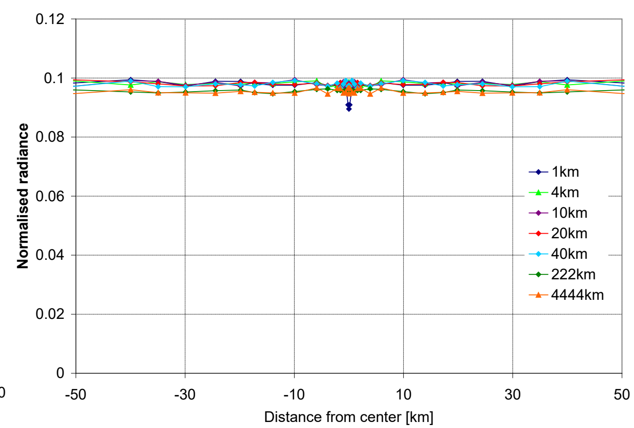
plume concentrations



AMF for plume scans



radiances for plume scans



(maximum VCD: 1e19)

=>for lower concentrations the effect is weaker

3) Saturation effects (for strong SO_2 absorption)

-simulations for SO_2 plumes of different horizontal extensions are performed

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simulations for 332 nm

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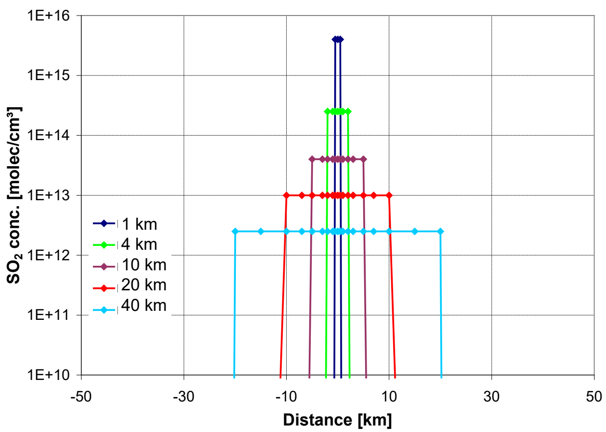
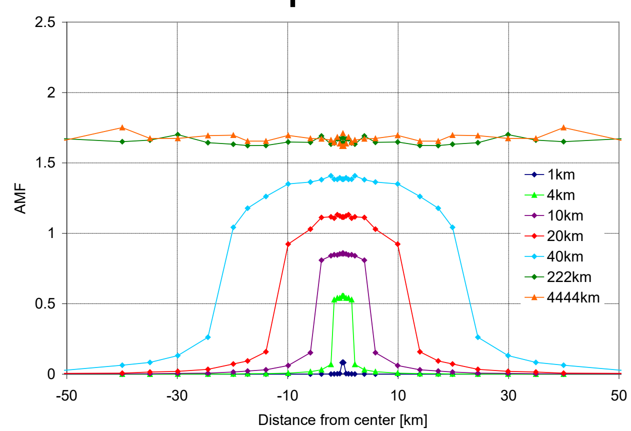
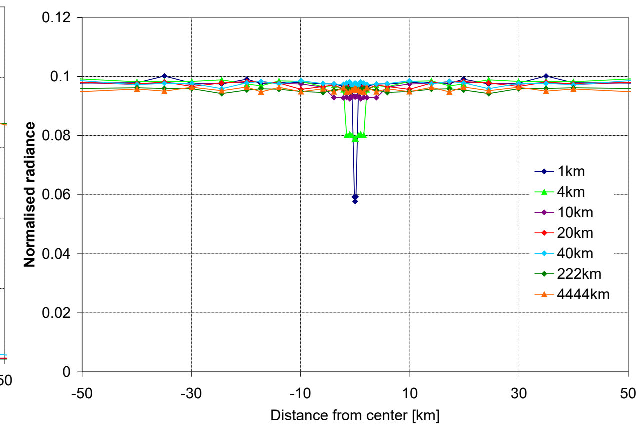


AMF for plume scans



radiances for plume scans



(maximum VCD: 4e20)

=> for larger wavelengths the effect is weaker

Effect 1: Horizontal light paths

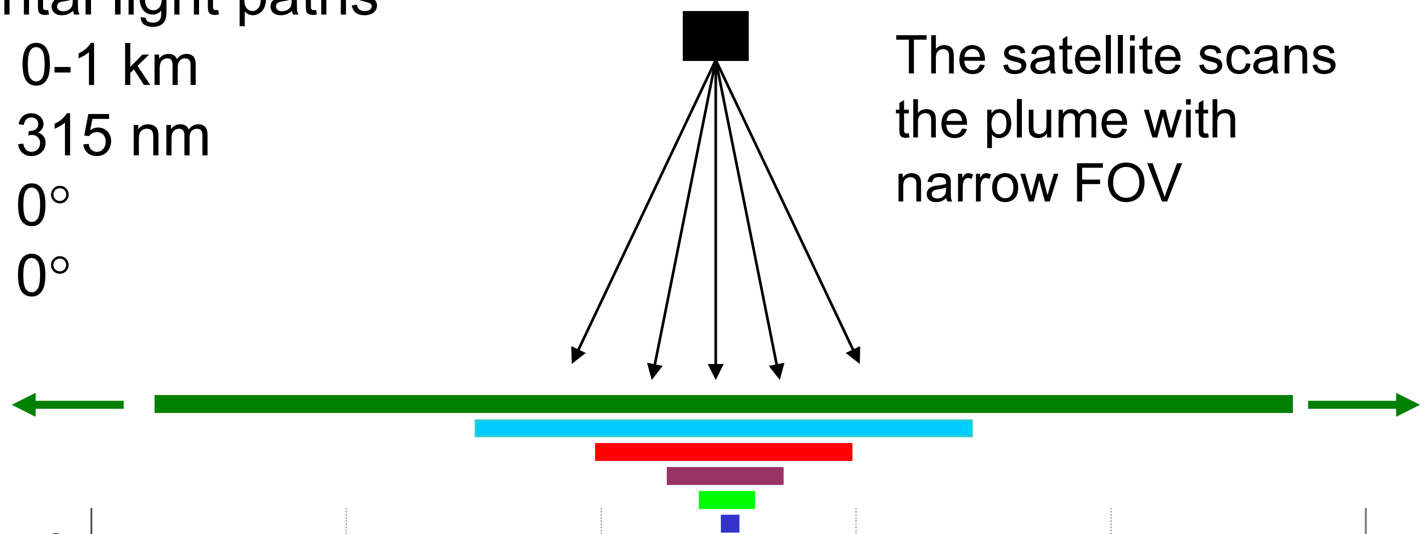
Plume altitude: 0-1 km

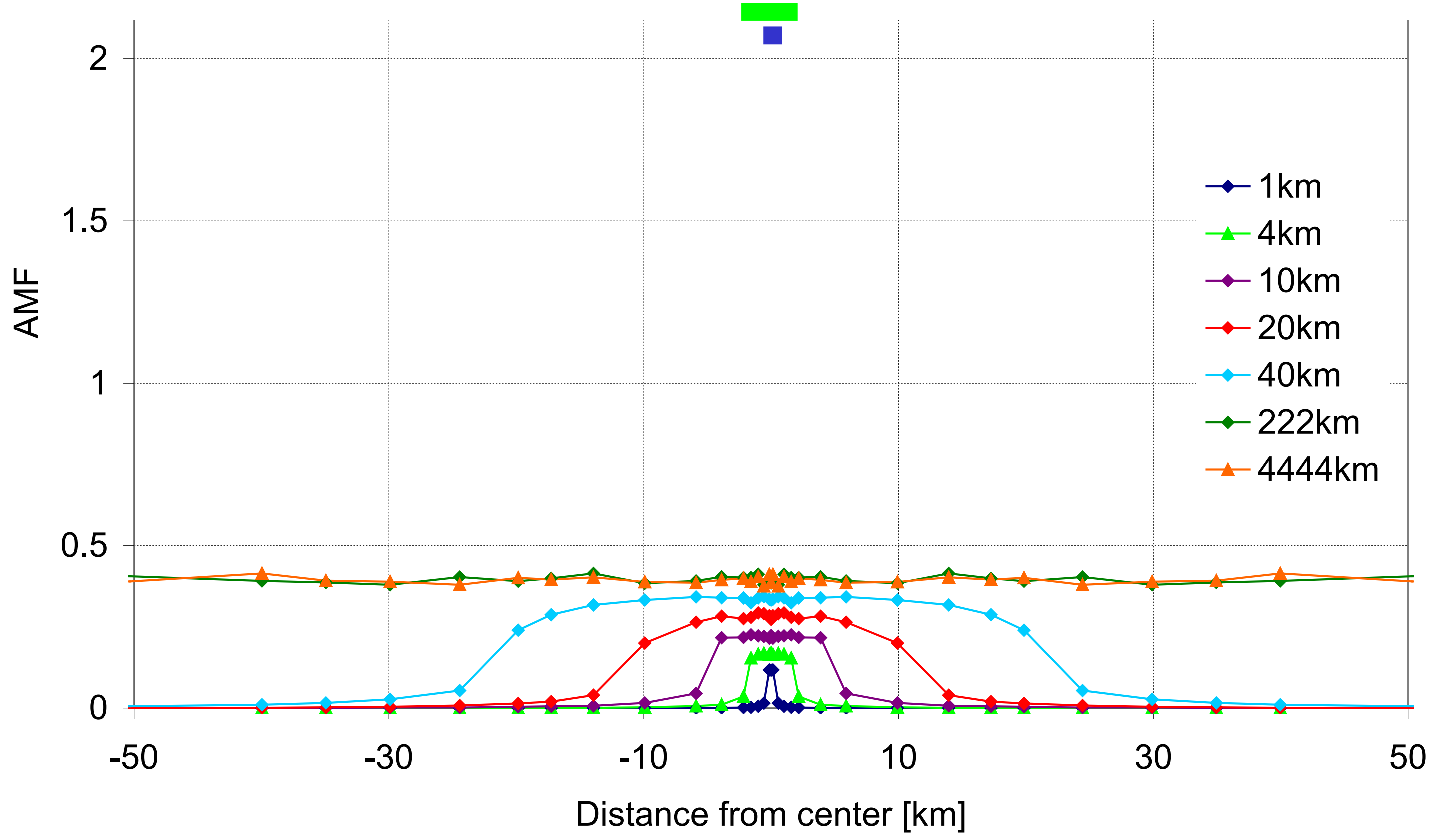
Wavelength: 315 nm

SZA: 0°

VZA: 0°

The satellite scans the plume with narrow FOV





=> much lower values (shielding effect)

=> even more smearing out

Effect 1: Horizontal light paths

Plume altitude: 10-10 km

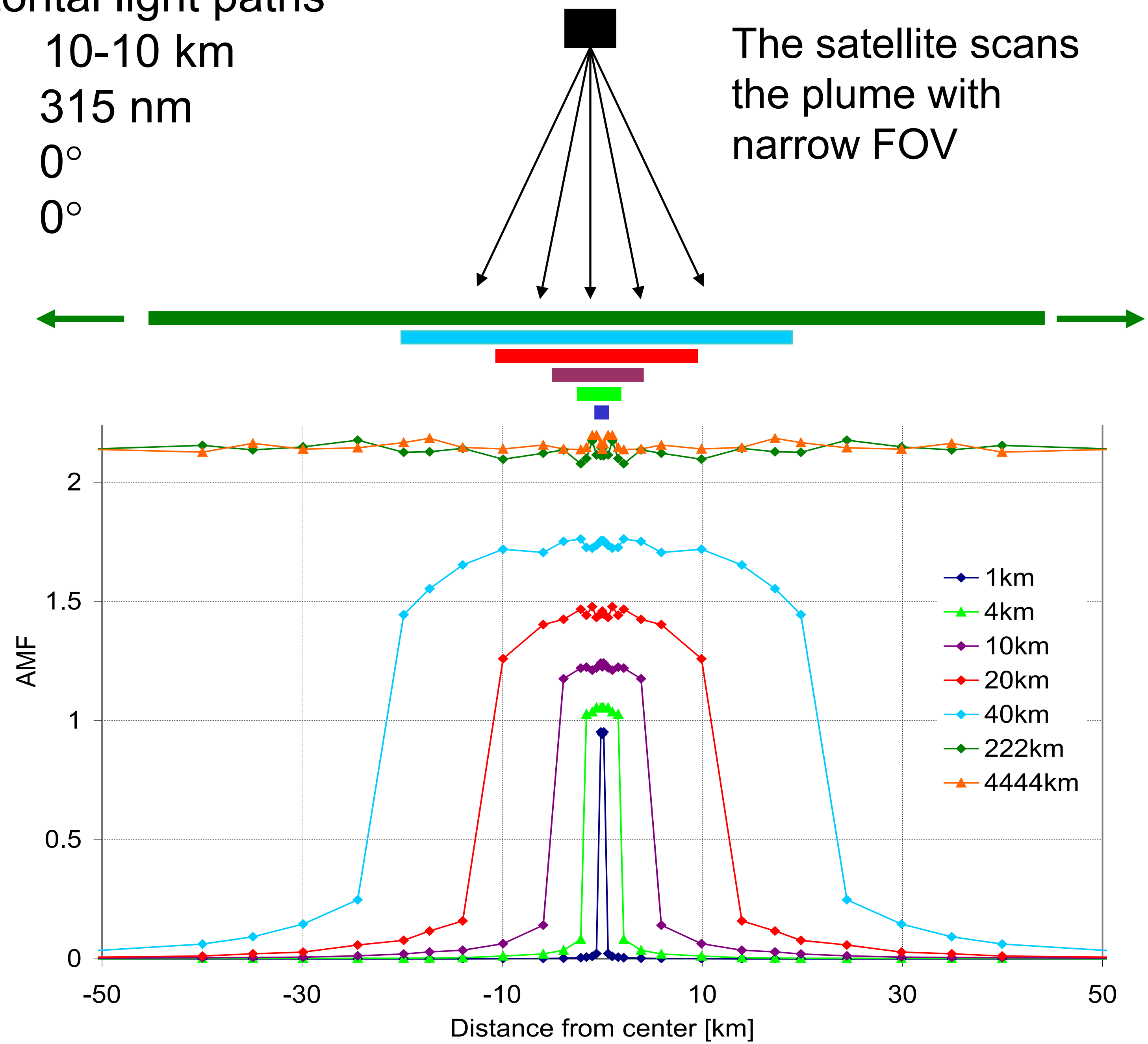
Wavelength: 315 nm

SZA: 0°

VZA: 0°

The satellite scans the plume with narrow FOV

=> much less shielding effect



Effect 1: Horizontal light paths

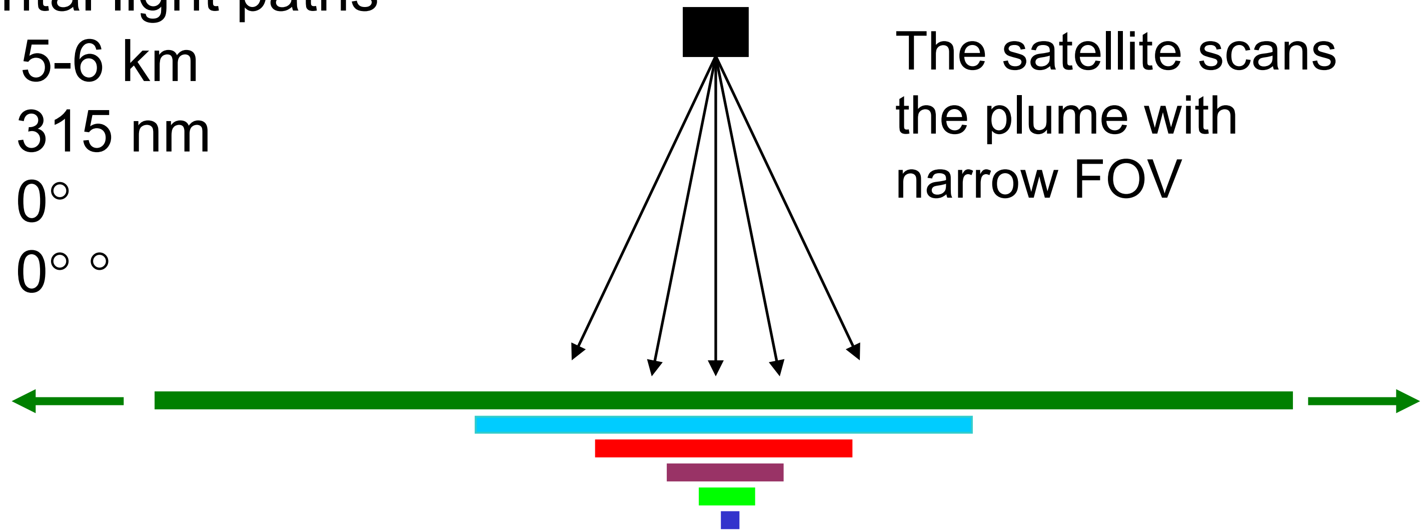
Plume altitude: 5-6 km

Wavelength: 315 nm

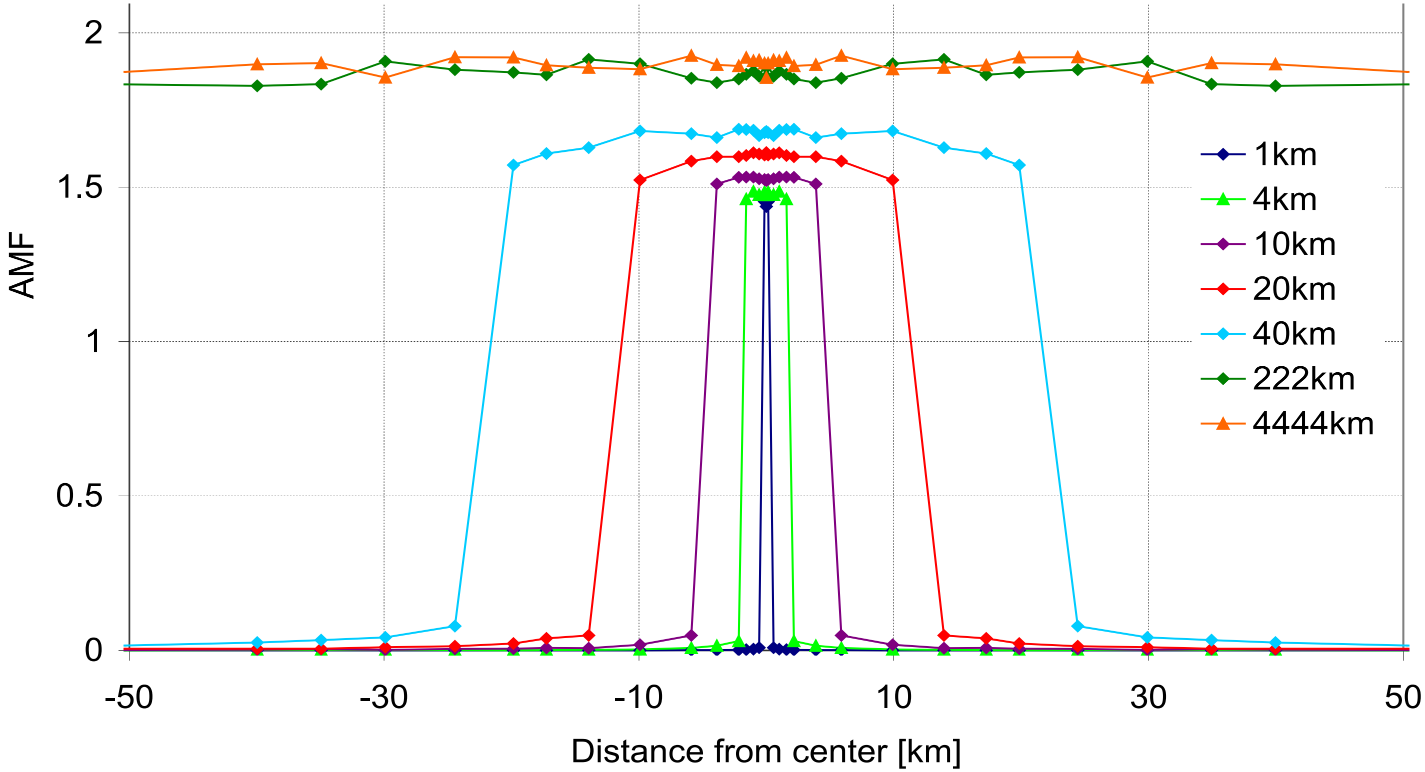
SZA: 0°

VZA: 0° °

The satellite scans the plume with narrow FOV



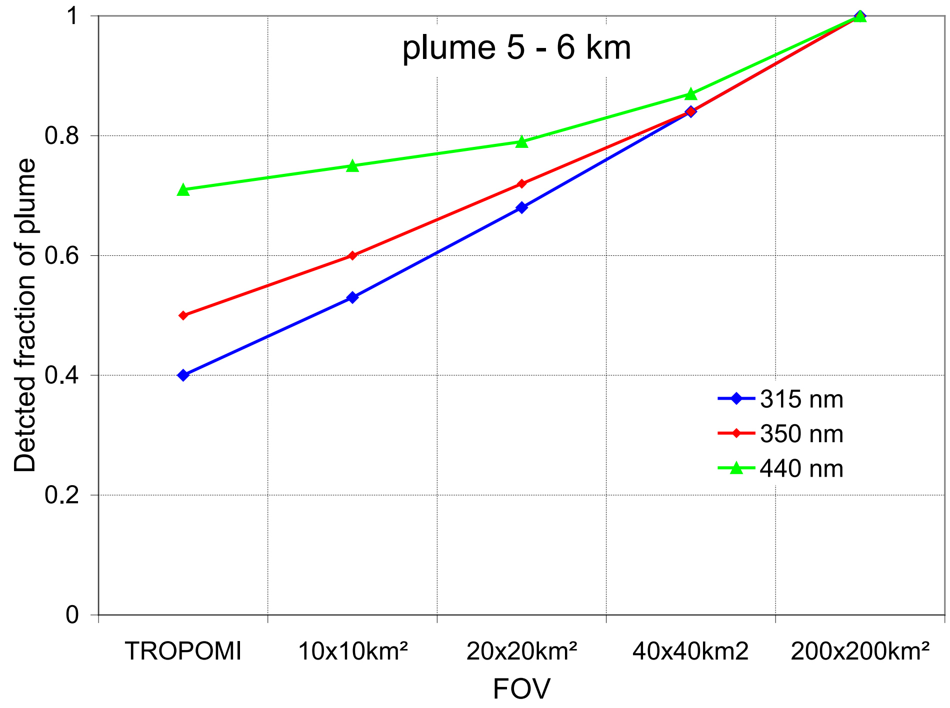
=> much sharper edges



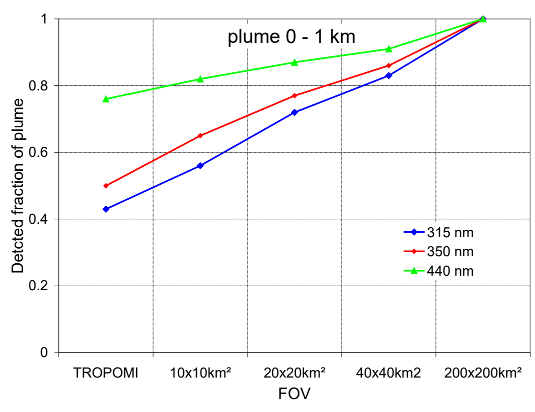
Effect 1: Horizontal light paths

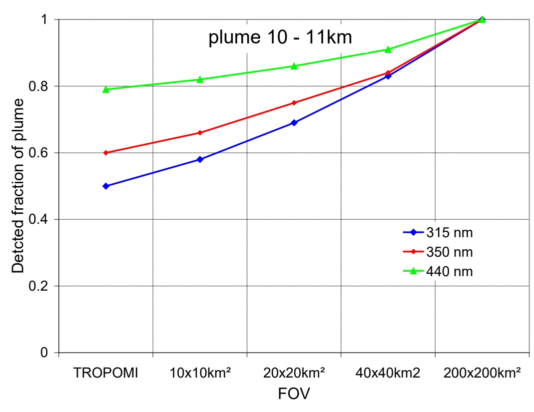
Fraction of detected plume molecules as function of the FOV for different wavelengths

Plume: 2 x 2 km²

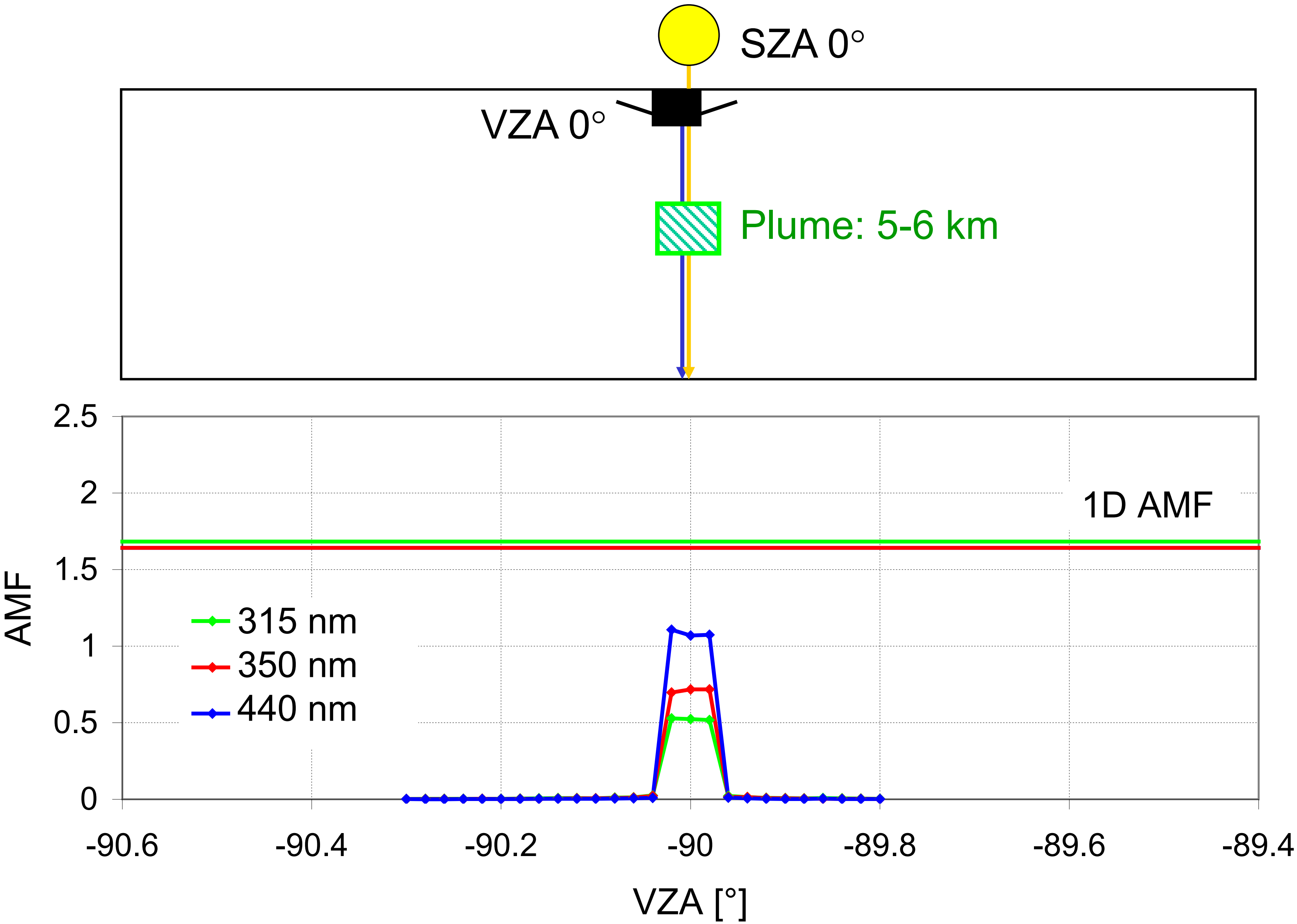


Similar results for other layer heights

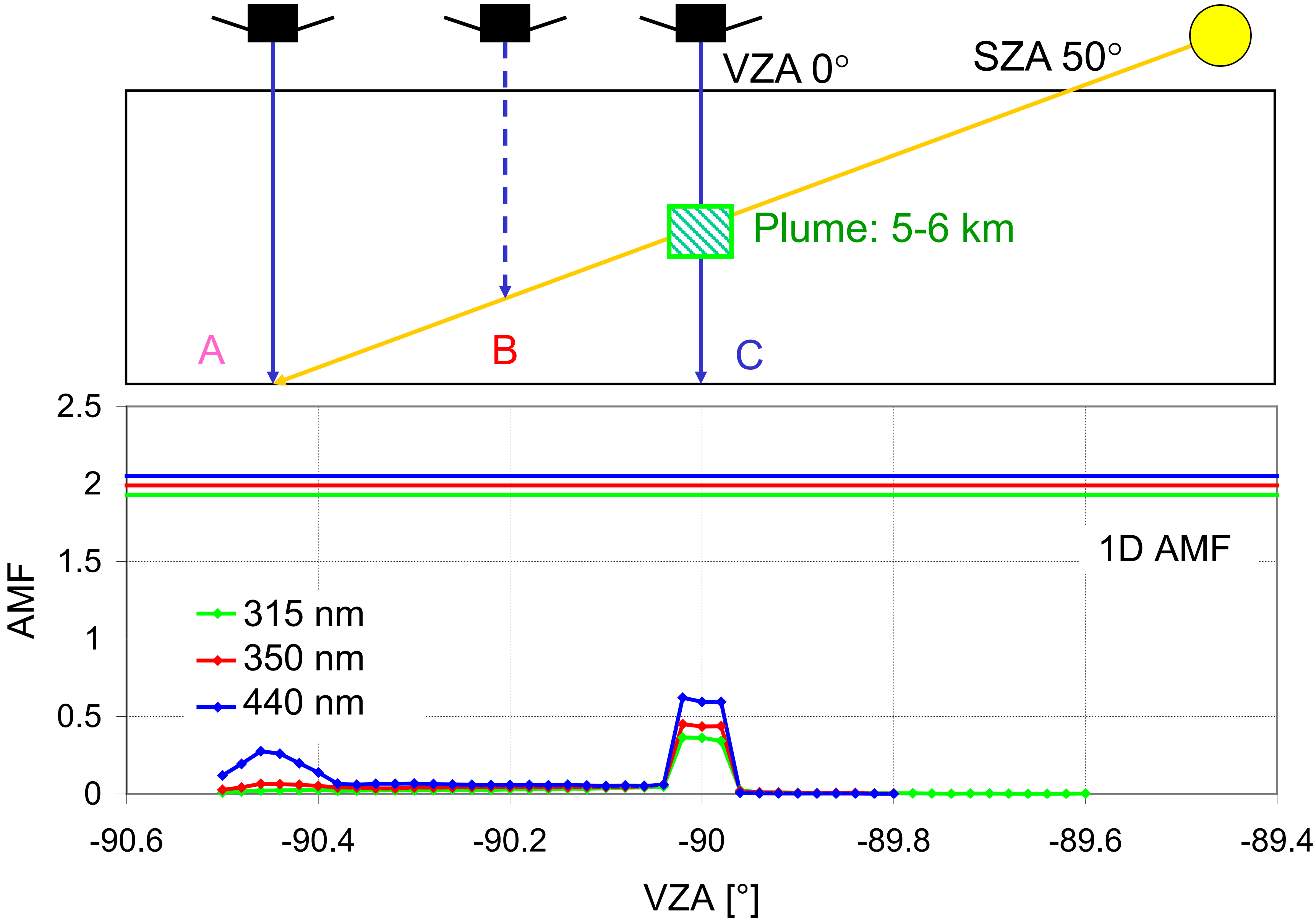




horizontal_light_paths.xls



Etna_center_plume_O4_scan_SZA0_VZA_90_all_WL.xls

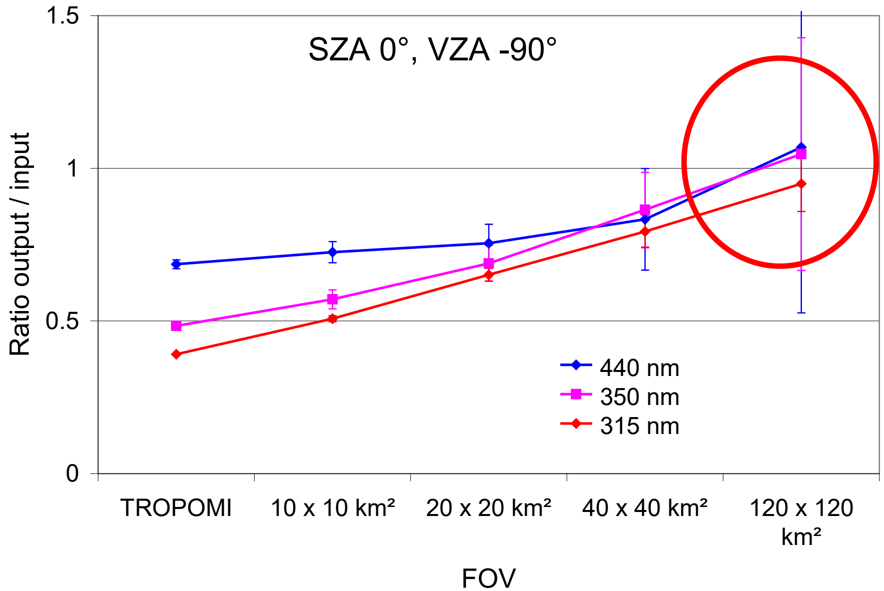


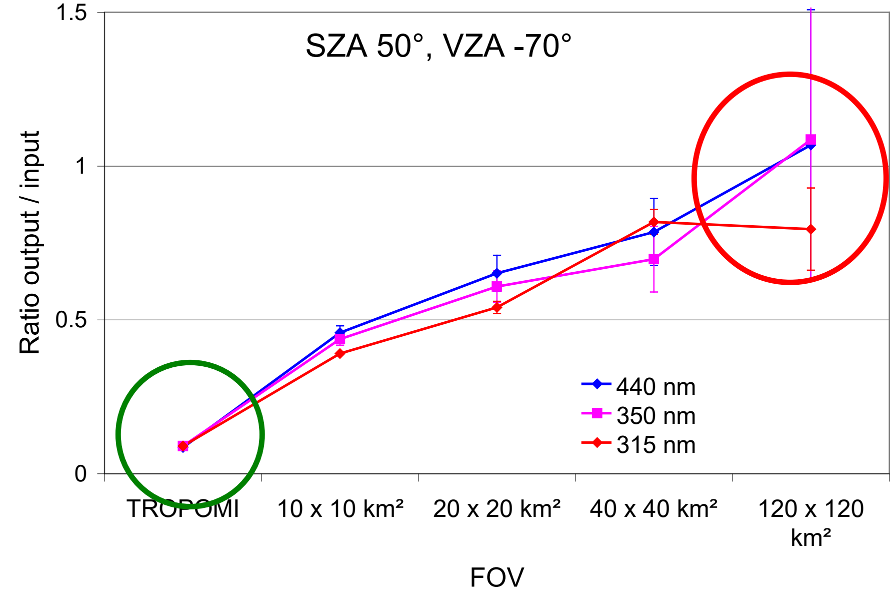
A: direct sun light crosses plume and is reflect at surface

B: direct sun light crosses plume and is scattered

C: line of sight crosses plume

Dependence of the ratio output / input on the FOV





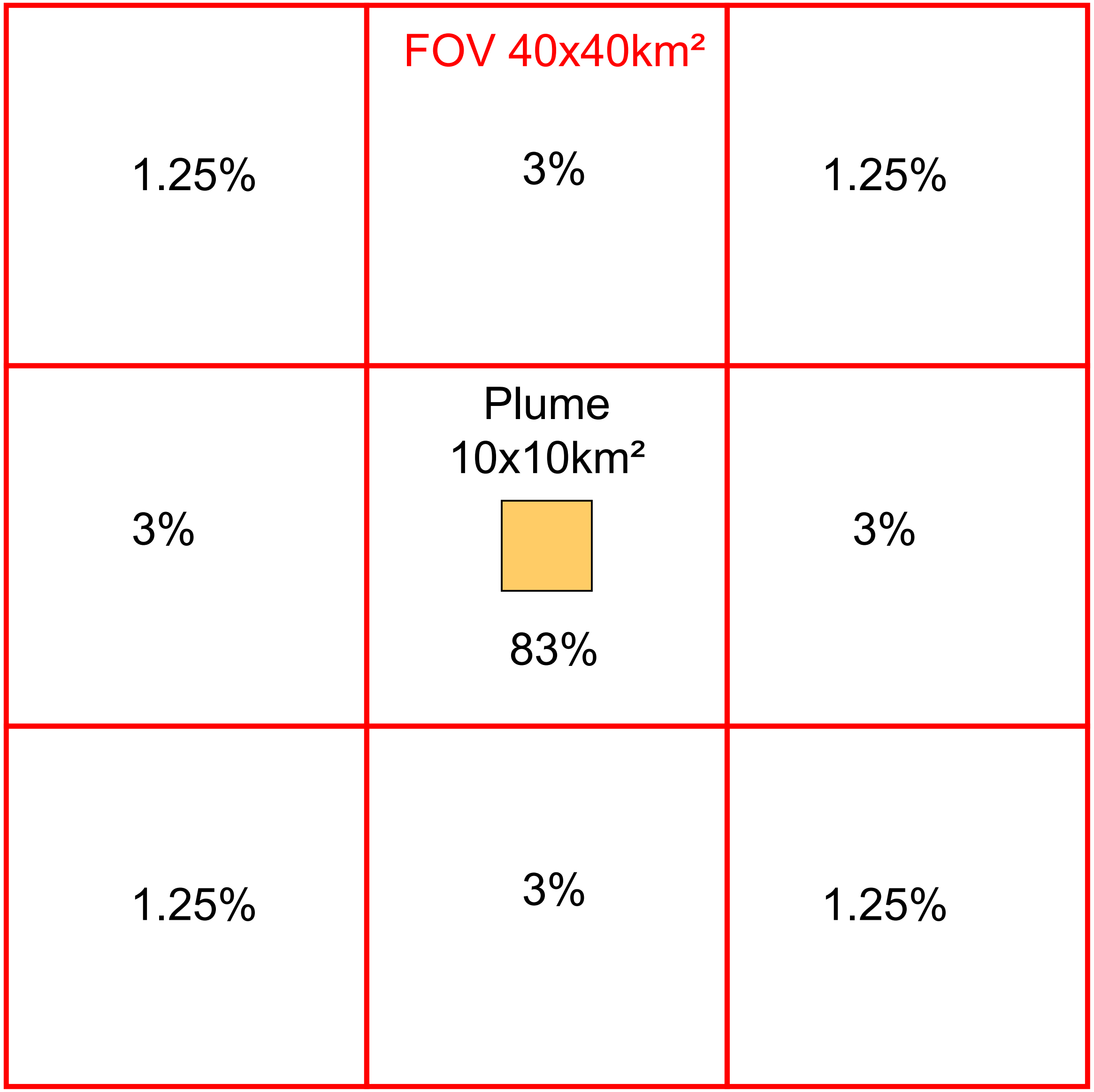
=> for large FOV the whole plume is seen (but the average trace gas absorption is very low.

=> in extreme cases the plume is not seen at the location where it is; instead a double plume is seen

=> the effect increases with plume altitude

Effect 1: Horizontal light paths

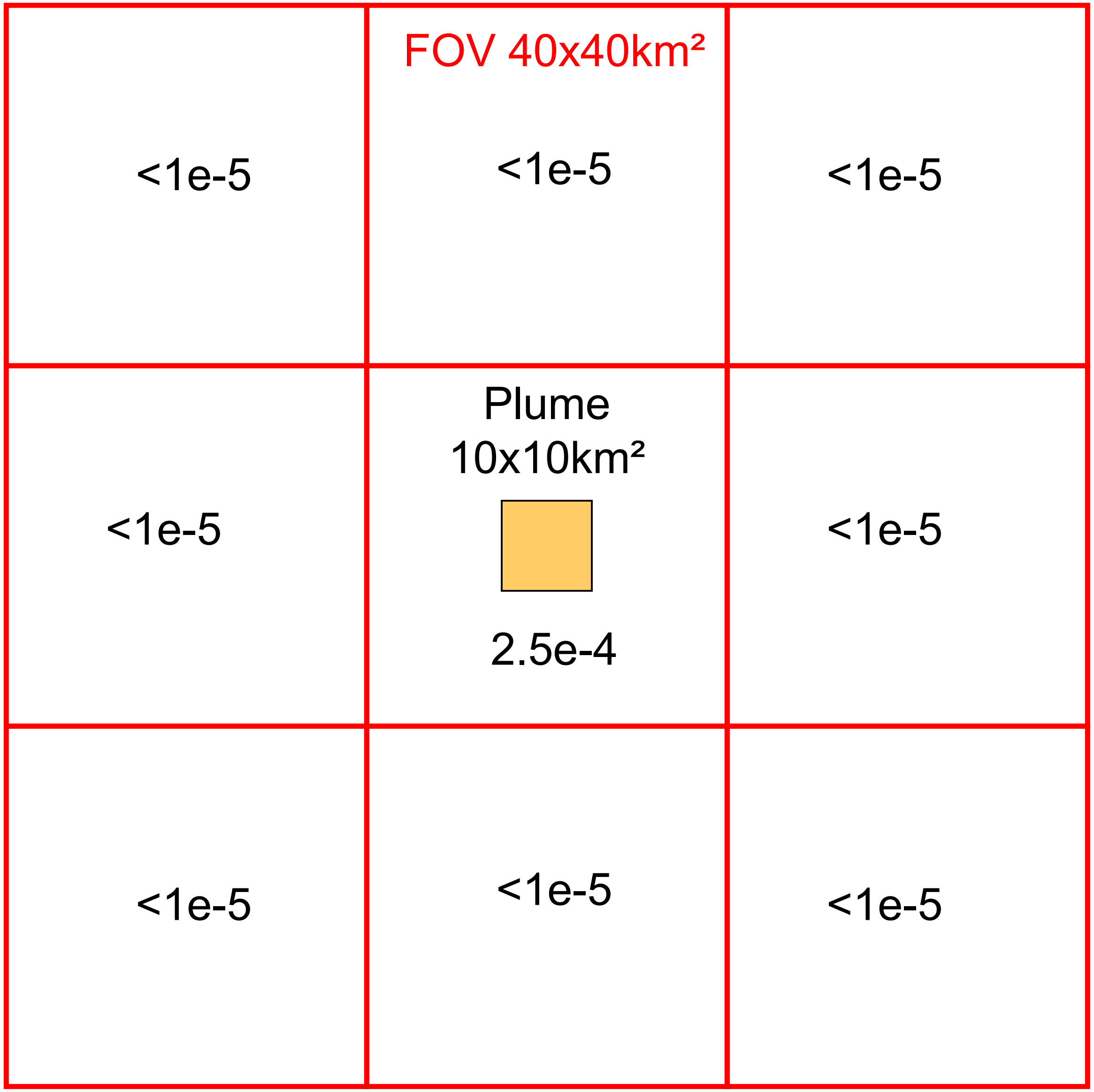
-can increased AMF ‚outside‘ the plume compensate for decrease ‚inside‘ the plume?



=> Total
= 100%

Effect 1: Horizontal light paths

-What about the absorption strength?



Assume a BrO VCD of 1e14 molec/cm² in the plume

=> the signal for all pixels outside the center pixel is below the detection limit:

only ~ 83% of the plume will be detected

1) Effect of horizontal light paths

How long do photons travel?

e-folding lengths for horizontal light paths at different wavelengths and altitudes (only Rayleigh scattering):

wavelength:	altitude	315nm	350nm	440nm
	0-1km:	9 km	16 km	30 km
	5-6km:	14 km	25 km	47 km
	10-11km:	35 km	66 km	122 km

=> similar distances as the size of volcanic plumes and the TROPOMI pixel size

(in the presence of aerosols the light paths become (much) shorter)

Effects of aerosols

-aerosol interact with all 3D effects discussed before
-here we show the effects on horizontal light paths
-the other effects will be studied in the near future
-general assumption: aerosols and trace gases are in the same volume

Results for 315 nm and plume at 5-6 km

no aerosols | AOD 2, SSA 1 | AOD 2, SSA 0.8

AMF

radiance