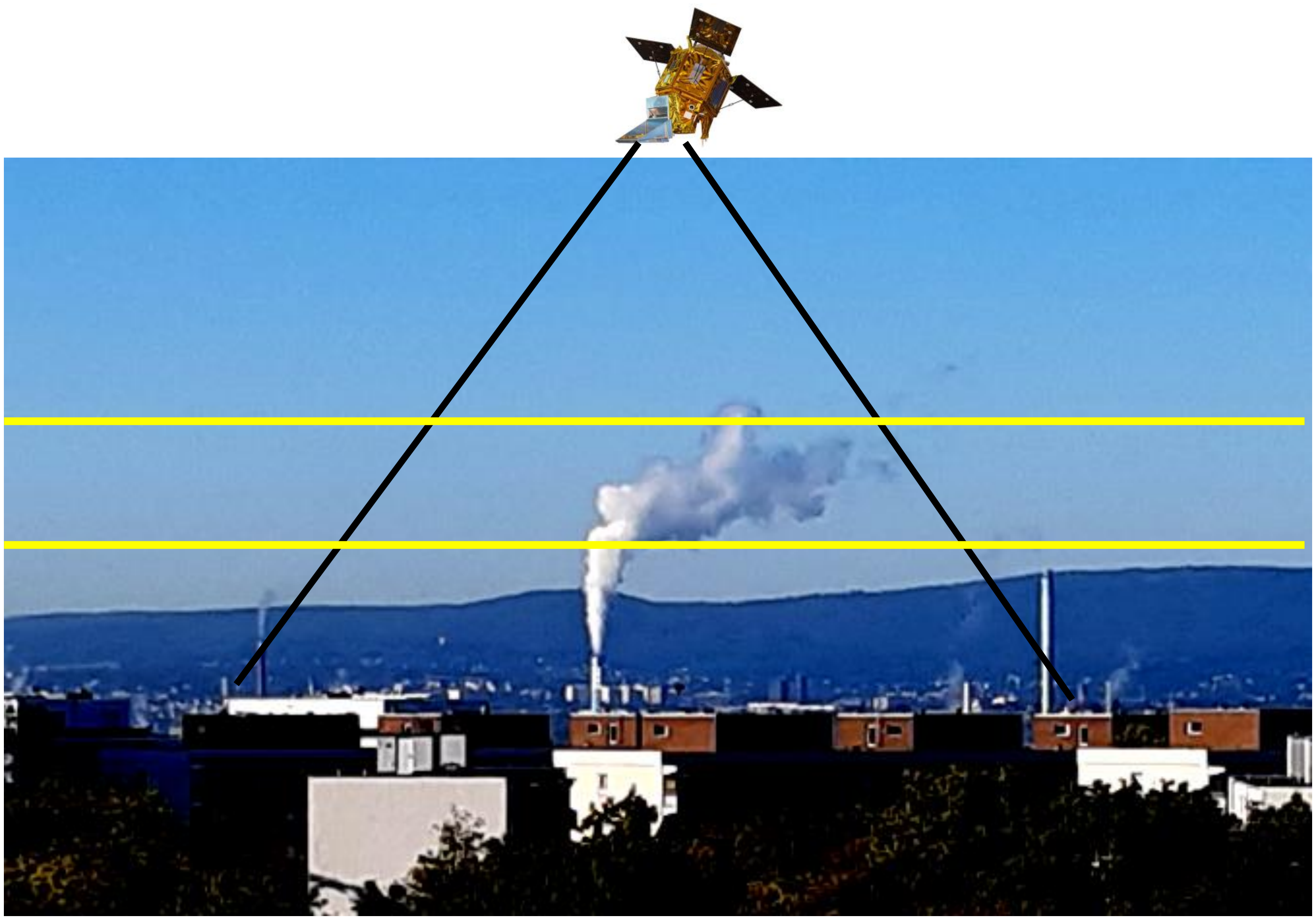
# Investigation of 3D-effects for S5P-TROPOMI observations of point source emissions

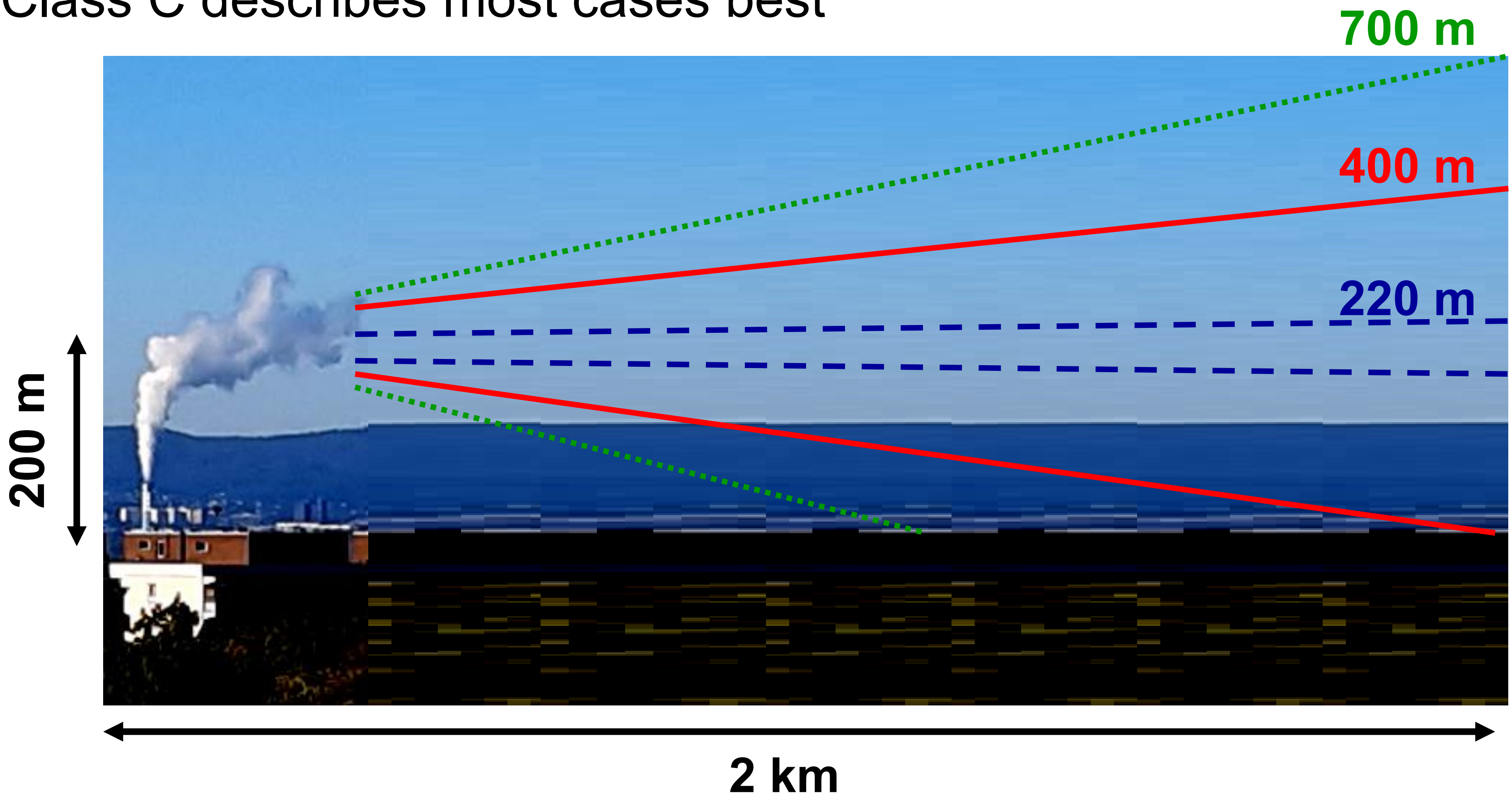
Thomas Wagner, Steffen Beirle
Max Planck Institute for Chemistry, Germany



We use the the plume characterisation according to Pasquill / Biggs (1973):

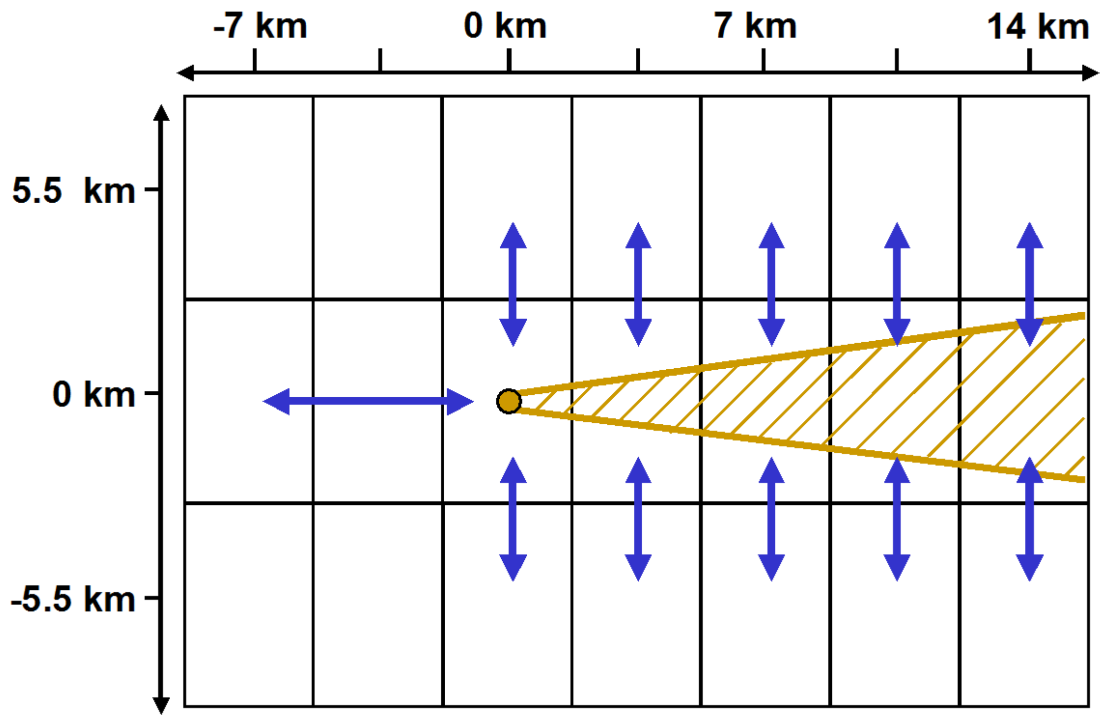
- class A: very unstable
- class C: slightly unstable
- class F: very stable

Class C describes most cases best



**Two main effects are investigated:**

A) effect of horizontal light paths




Pattern of TROPOMI pixels above point source

- light from the pixels containing the plume is scattered outside
- light from outside the pixels is scattered inside

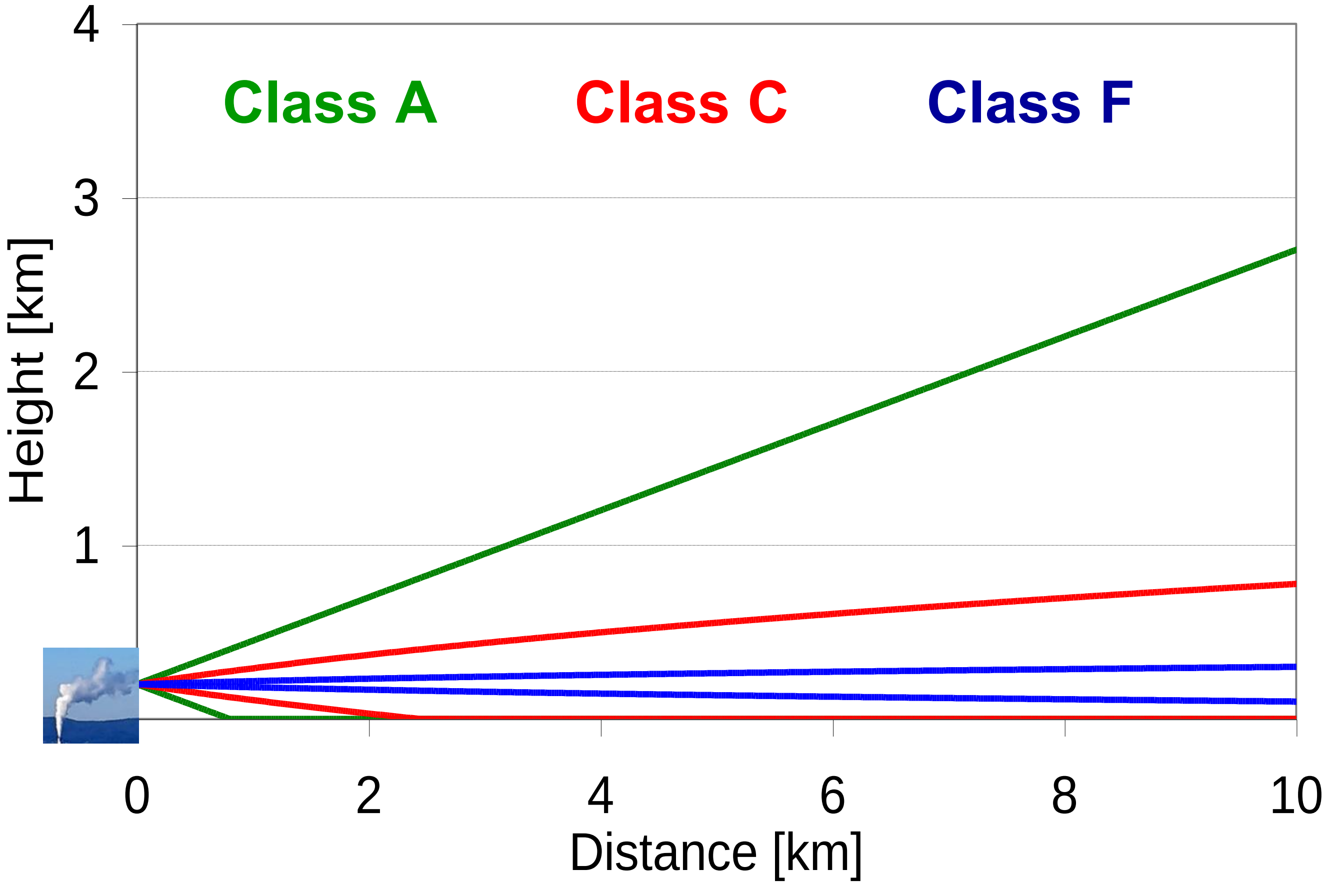
=> The absorption signal of the ‘plume pixels’ is weakened

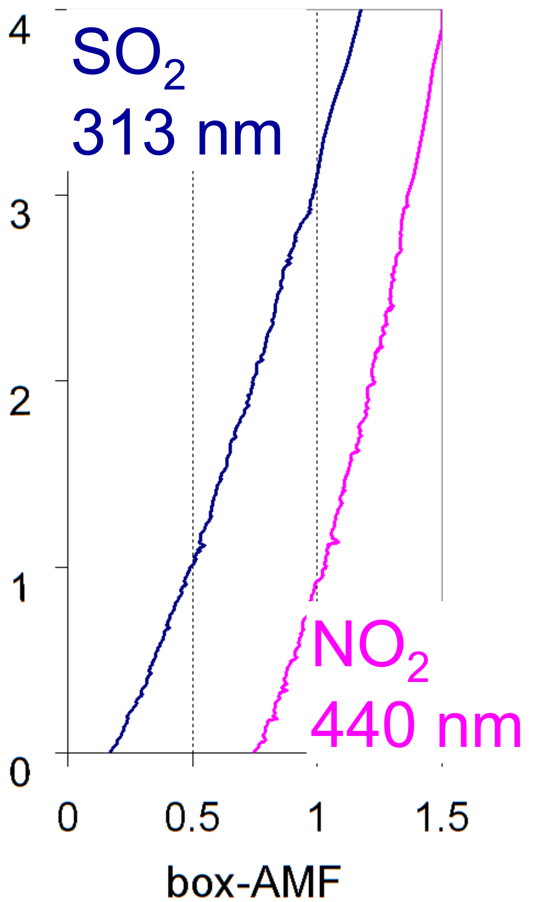
=> The absorption signal of the outside pixels is > 0

**Two main effects are investigated:**

B) effect of increasing pume height with distance

=> The sensitivity of the measurement increases with increasing distance from the source



Both effects are studied using the 3D Monte-Carlo model **TRACY-2**

Developed by Tim Deutschmann, Uni-Heidelberg

(see Wagner et al., ACP, 2007)

-3D-distributions of trace gases and aerosols

-suface topography

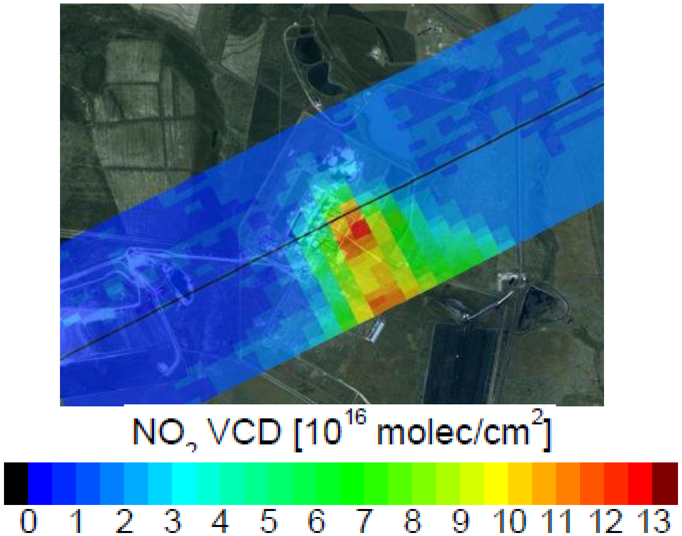
In this study:

- 3D trace gas plumes
- 1D aerosol scenarios:
  - AOD: 0.1, 0.3, 0.5, 1.0
  - layer heigts: 200 m, 500 m, 1000 m, 2000 m

  => **standard scenario: AOD: 0.3, 1000 m**

$NO_2$ and $SO_2$ VCDs are taken from existing measurements

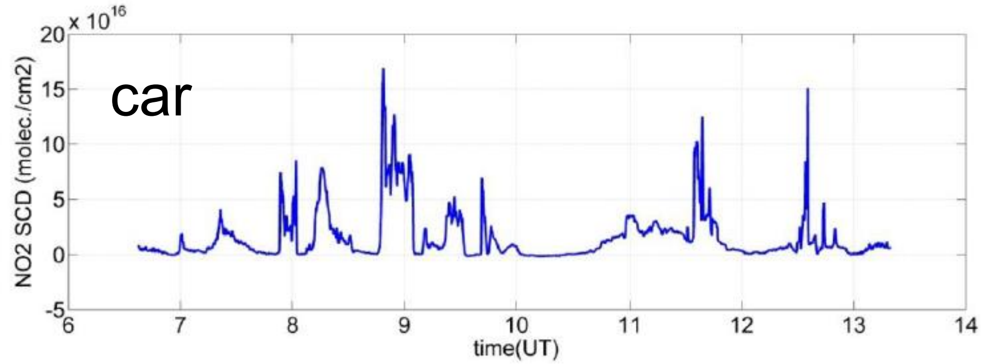
# $NO_2$ plume VCDs from existing measurements

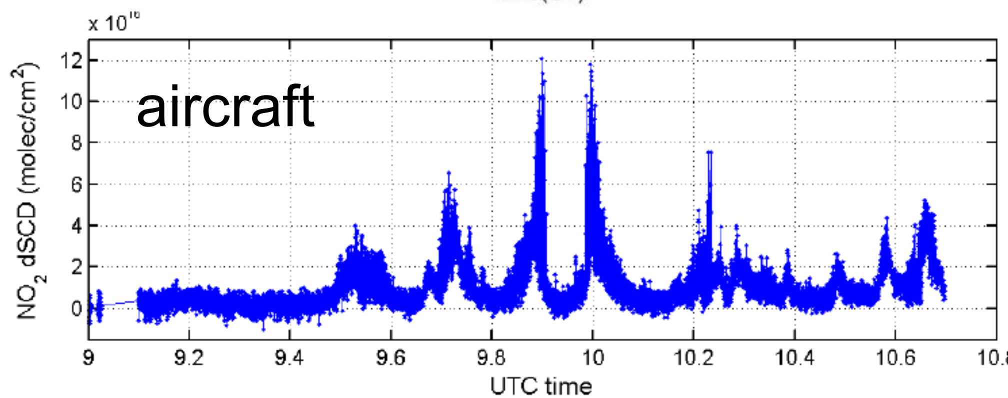



$NO_2$ VCD around the Majuba power plant (South Africa)

Heue et al., ACP, 2008

A reference cross section of 200m x 200m with a $NO_2$ VCD of 1e17 molec/cm² is chosen in this study.

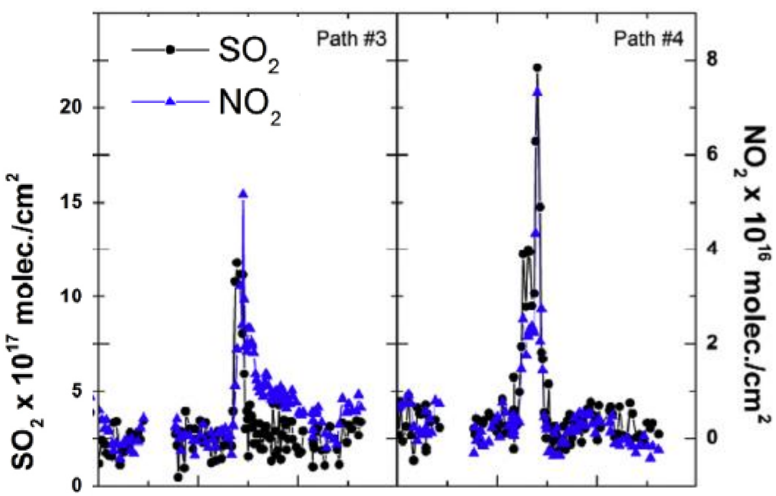



DOAS Measurements in the Jiu Valley (Romania) during the AROMAT-2 campaign.

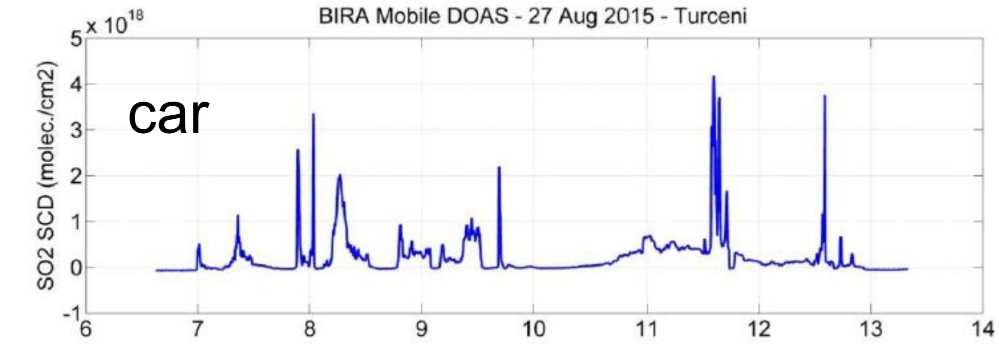
AROMAT-II Final Report, https://earth.esa.int/eogateway/documents/20142/37627/AROMAT-2-Final-Report.pdf

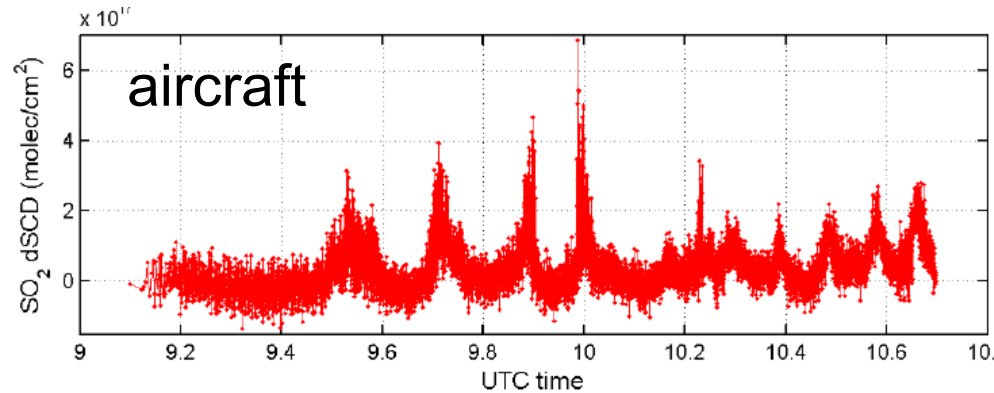
# $SO_2$ plume VCDs from existing measurements




$SO_2$ VCD around the Central Batlle power plant (Uruguay)

Frins et al., Atm. Env., 2014




A reference cross section of 200m x 200m with a $SO_2$ VCD of 4e17 or 4e18 molec/cm² is chosen in this study.

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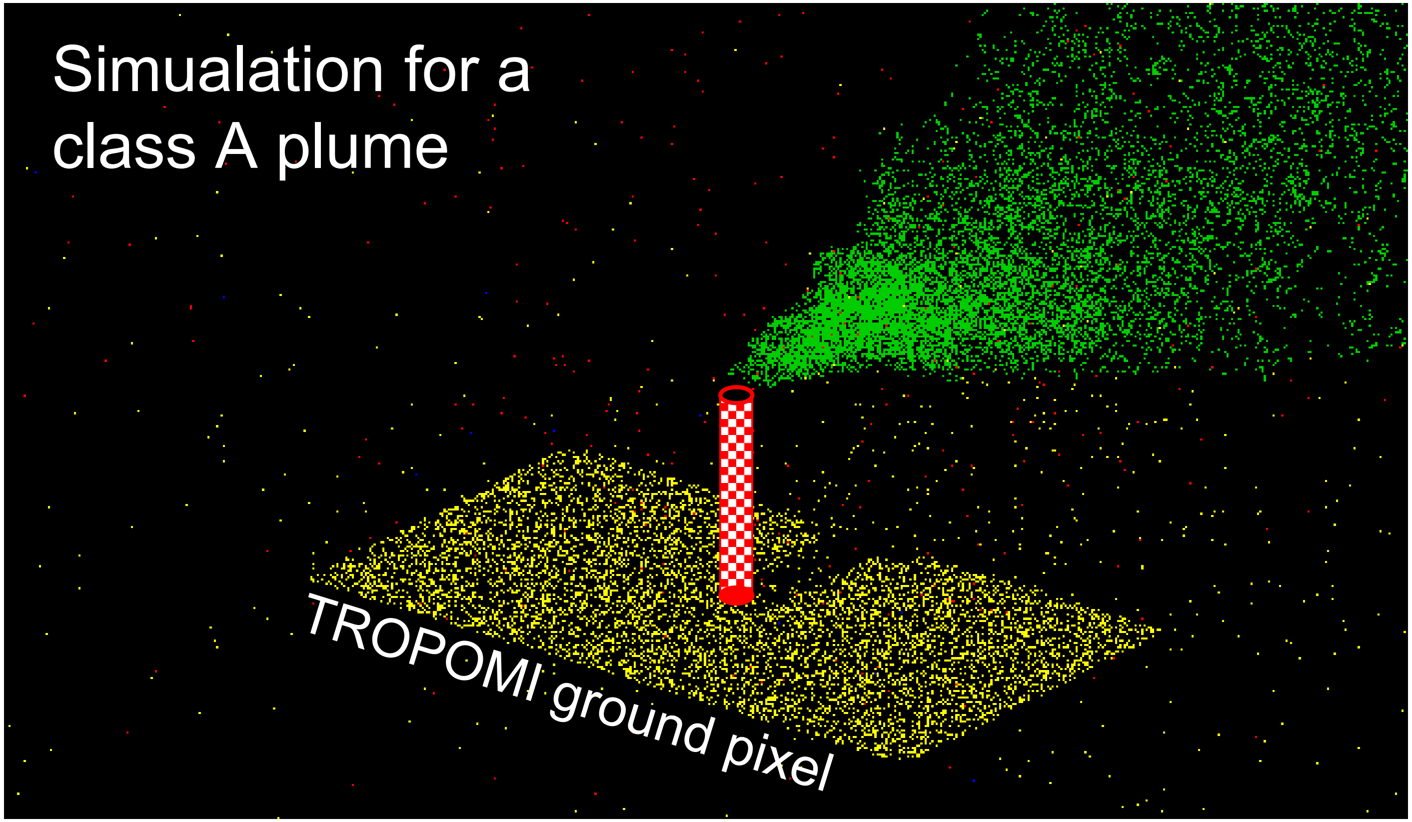
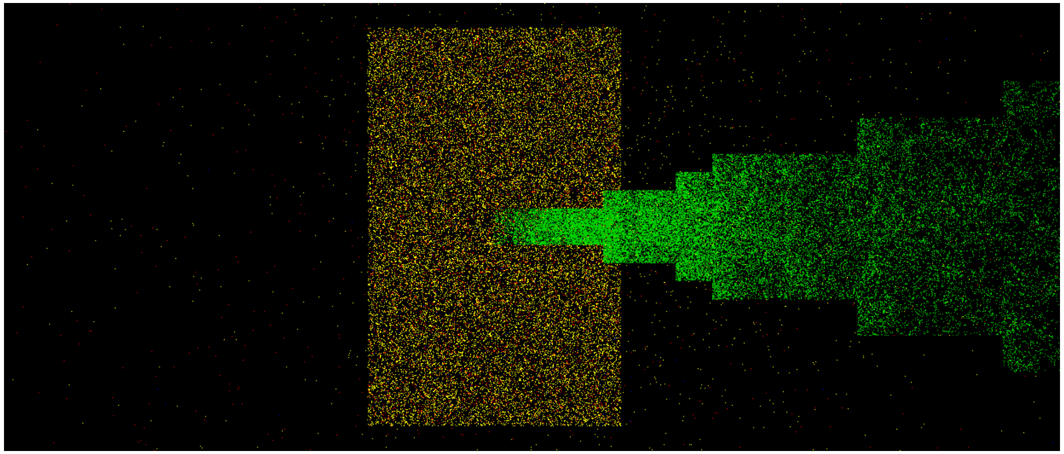
AROMAT-II Final Report, https://earth.esa.int/eogateway/documents/20142/37627/AROMAT-2-Final-Report.pdf

Both effects are studied using the 3D Monte-Carlo model **TRACY-2**

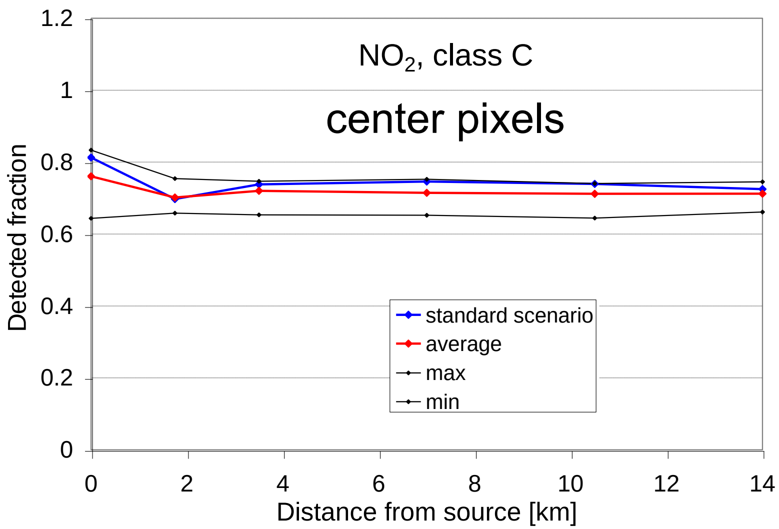


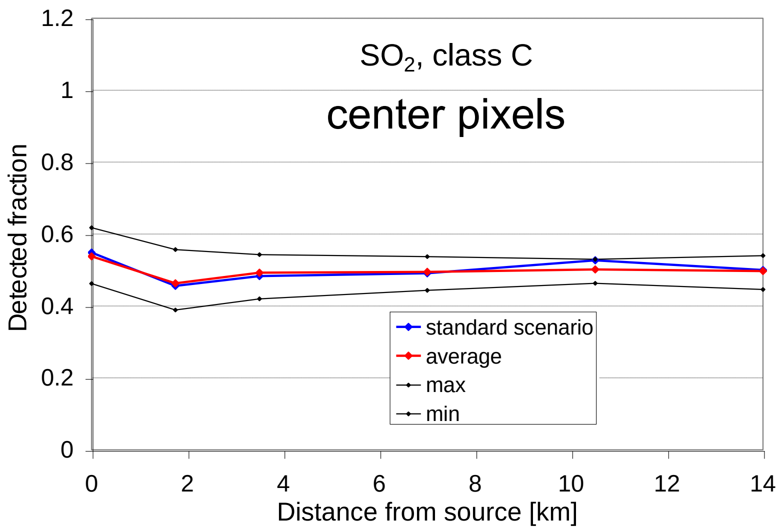



a simplified rectangular cross section is used

# A) effect of horizontal light paths

- 3D simulations are performed
- for a selected TROPOMI pixel, $I/I_o$ are simulated
- with the trace gas cross section, the SCD is derived
- the VCD is obtained by divison by the **corresponding 1D AMF***
- multiplcation with the pixel area yields the number of molecules
- the ratio to the input value yields the 'detected fraction'



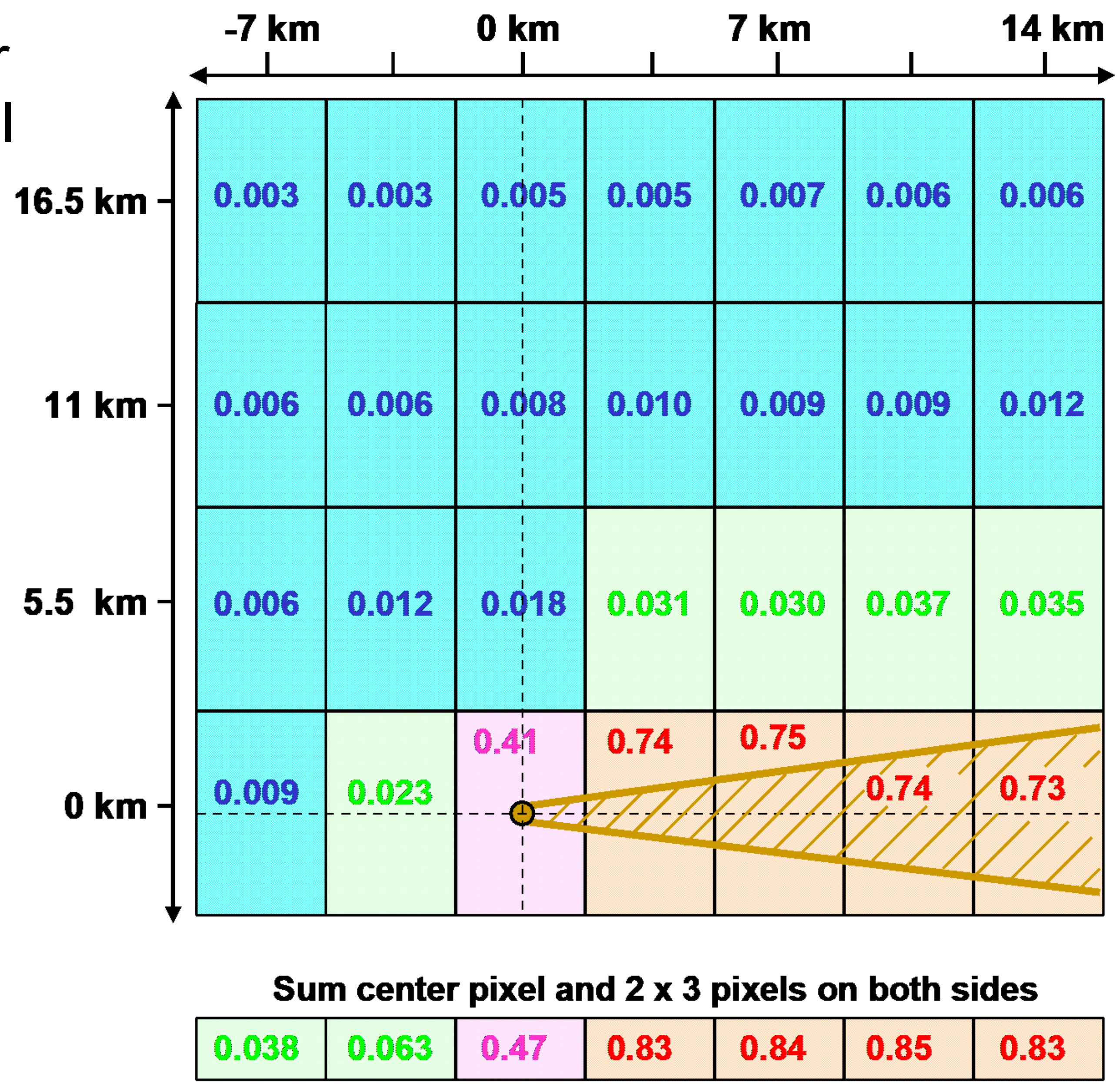




***AMF for the same (varying) altitude range of the plume**

# A) effect of horizontal light paths

Detected fraction for individual TROPOMI pixels

$NO_2$, standard scenario



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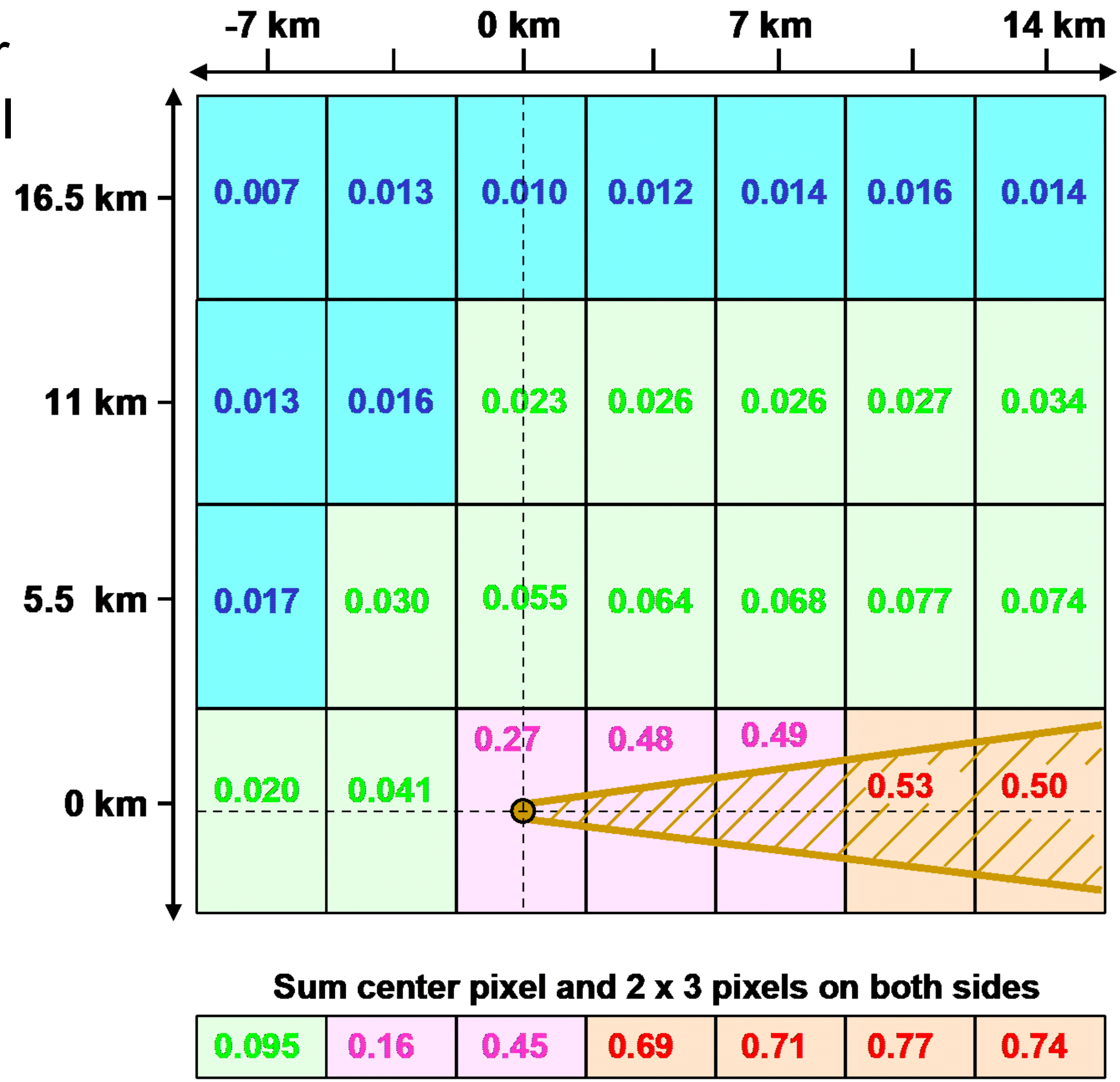
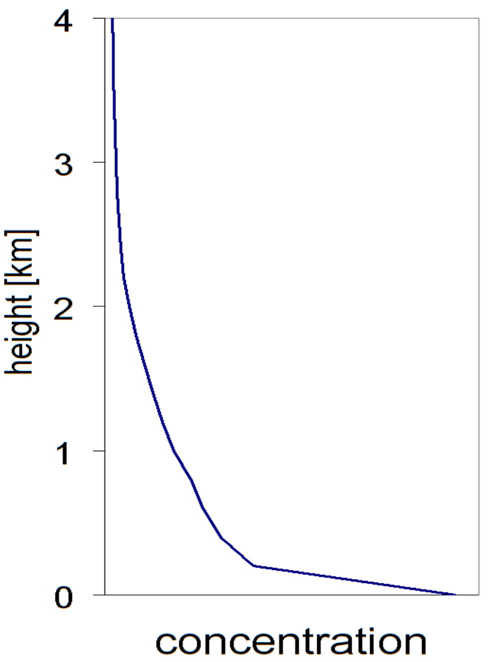


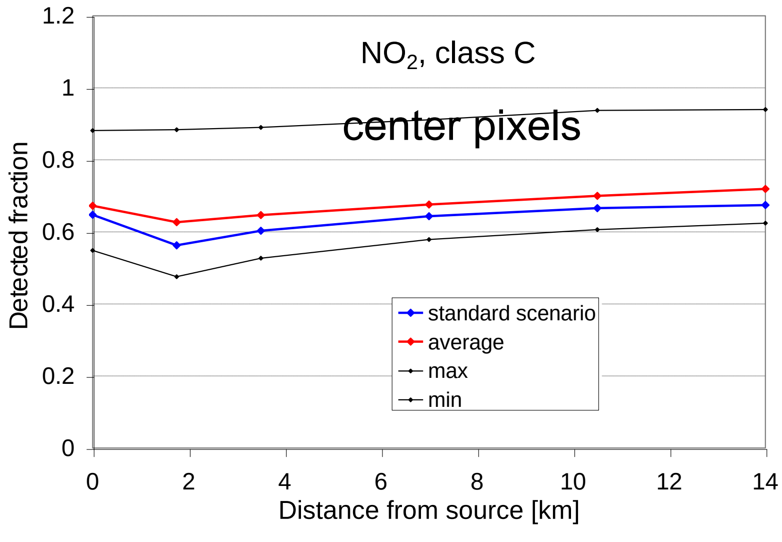
## B) increasing pume height with distance

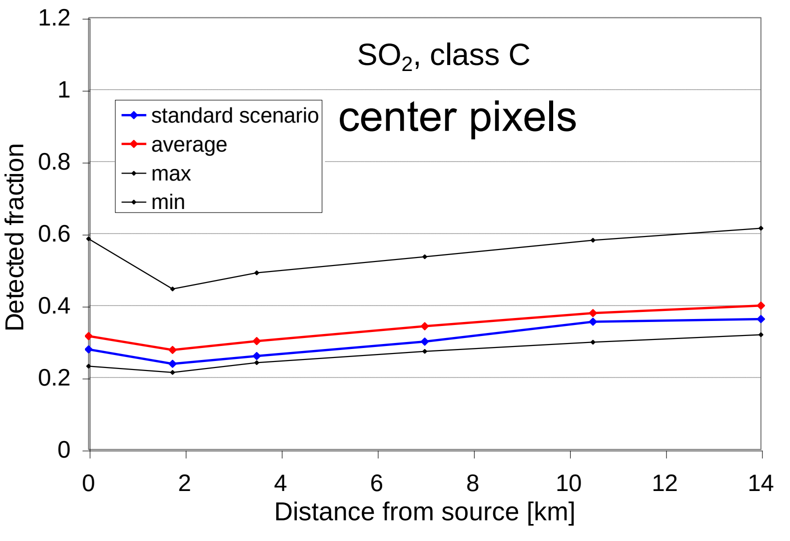
Now 'standard AMFs' are applied, calculated fo an urban profile (e.g. from Douros et al. (2022) for Paris from TM5:

**$NO_2$: 1.05**

**$SO_2$: 0.52**



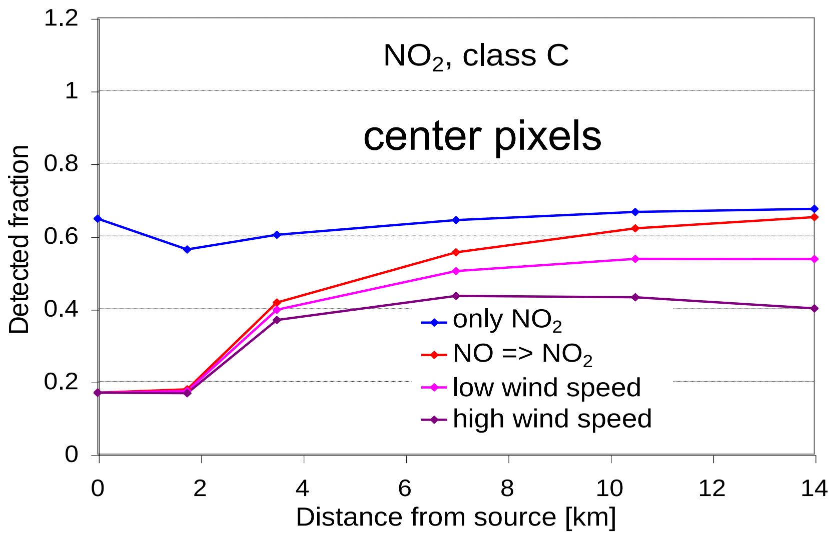



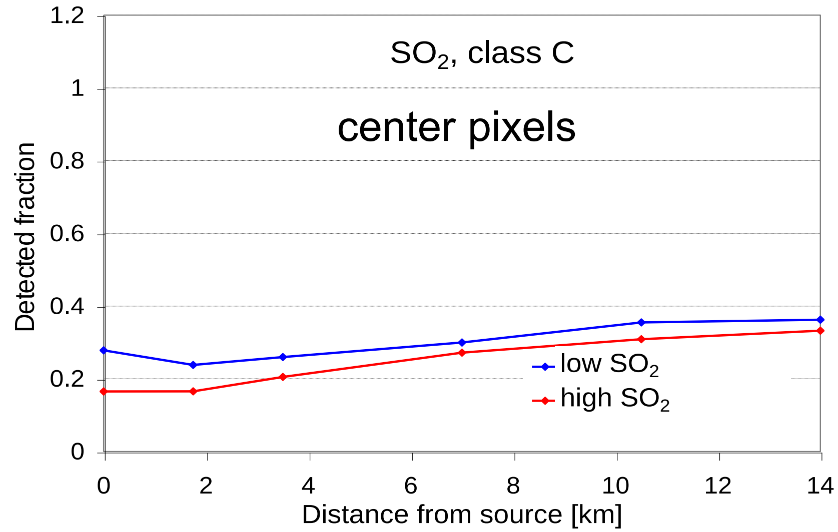

=> larger underestimation, larger spread

**Two additional effects are important and are also considered in this study:**

**$NO_2$:**
The conversion of NO to $NO_2$ along the plume direction*
(also destruction of $NO_x$ along the plume direction**)

**$SO_2$:**
The very strong absorption in the early (narrow) plume for strong emissions




*it is assumed that initially only NO is emitted
**assumed lifetime: 4 hours

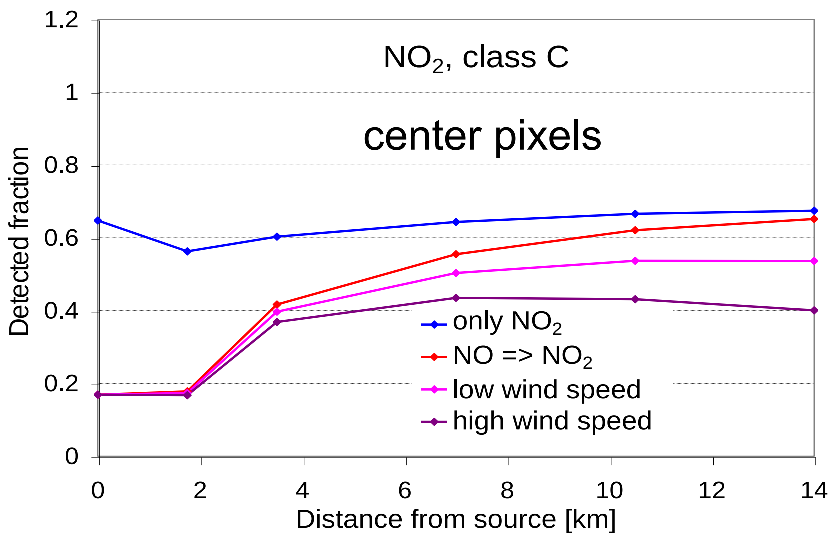
# Intermediate conclusions:

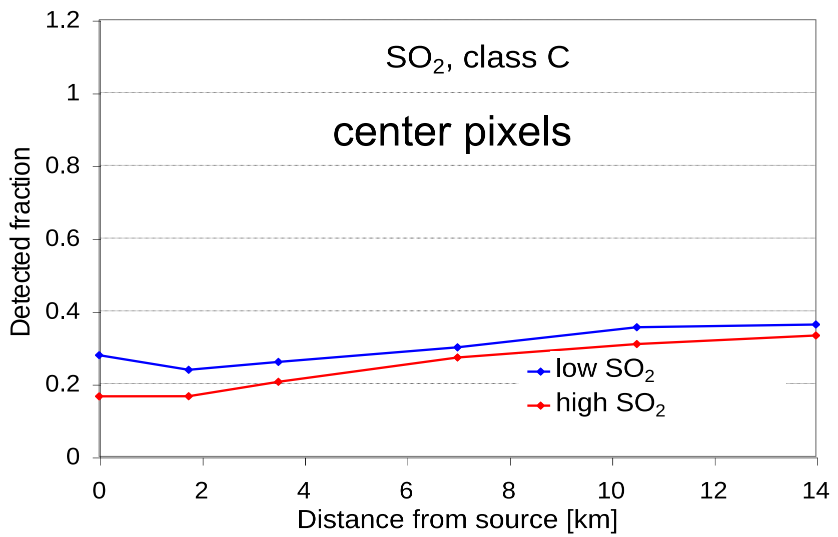
## $NO_2$:

- detected fraction above source is about 20 – 60%
- detected fraction at 10 km distance is about 40 – 60%

## $SO_2$:

- detected fraction directly above source is about 20 – 30%
- detected fraction at 10 km distance is about 35%




**=> What about more sofisticated techniques for the determination of emissions?**

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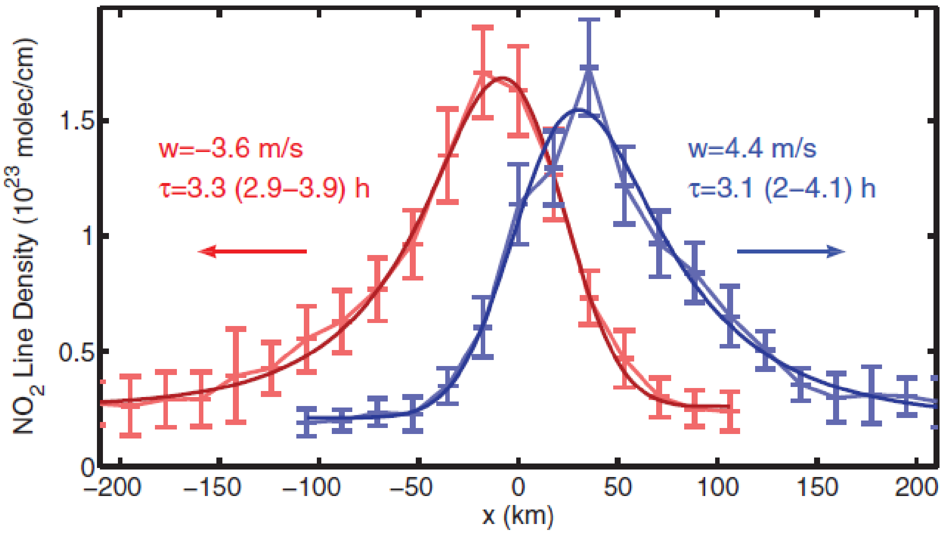
## A) Calculating downward decay for $NO_2$

$NO_2$ VCDs are averaged for the same wind direction. A model function is fitted to simultaneously determine the lifetime and the $NO_x$ emissions (Beirle et al., Science, 2011; Liu et al., ACP, 2022)



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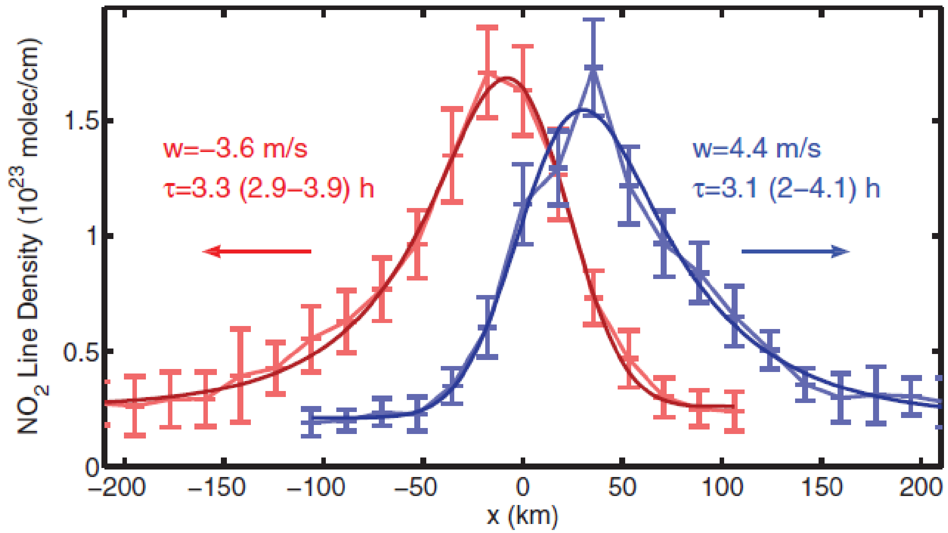



The same model function is applied to the simulated $NO_2$ VCDs as a function of the distance from the source. The following emissions are derived (class C, standard scenario):

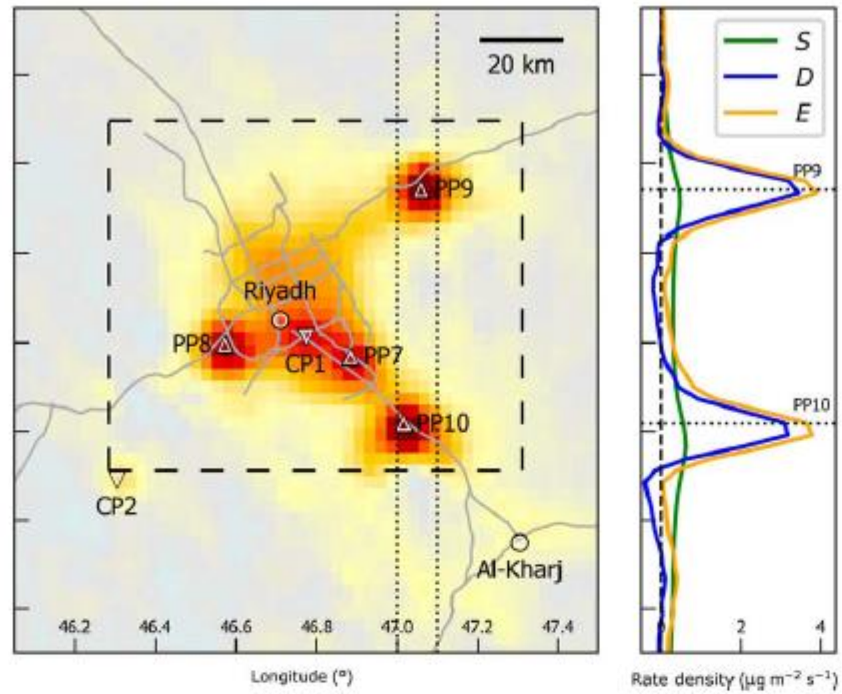
- $NO_2$ emitted, only center pixel: 58 %
- NO emitted, only center pixel: 52 %
- NO emitted, also neighbouring pixels: 61 %

(the lifetime was almost correctly retrieved)

=> What about more sofisticated techniques for the determination of emissions?

## B) Calculating the divergence of the flux

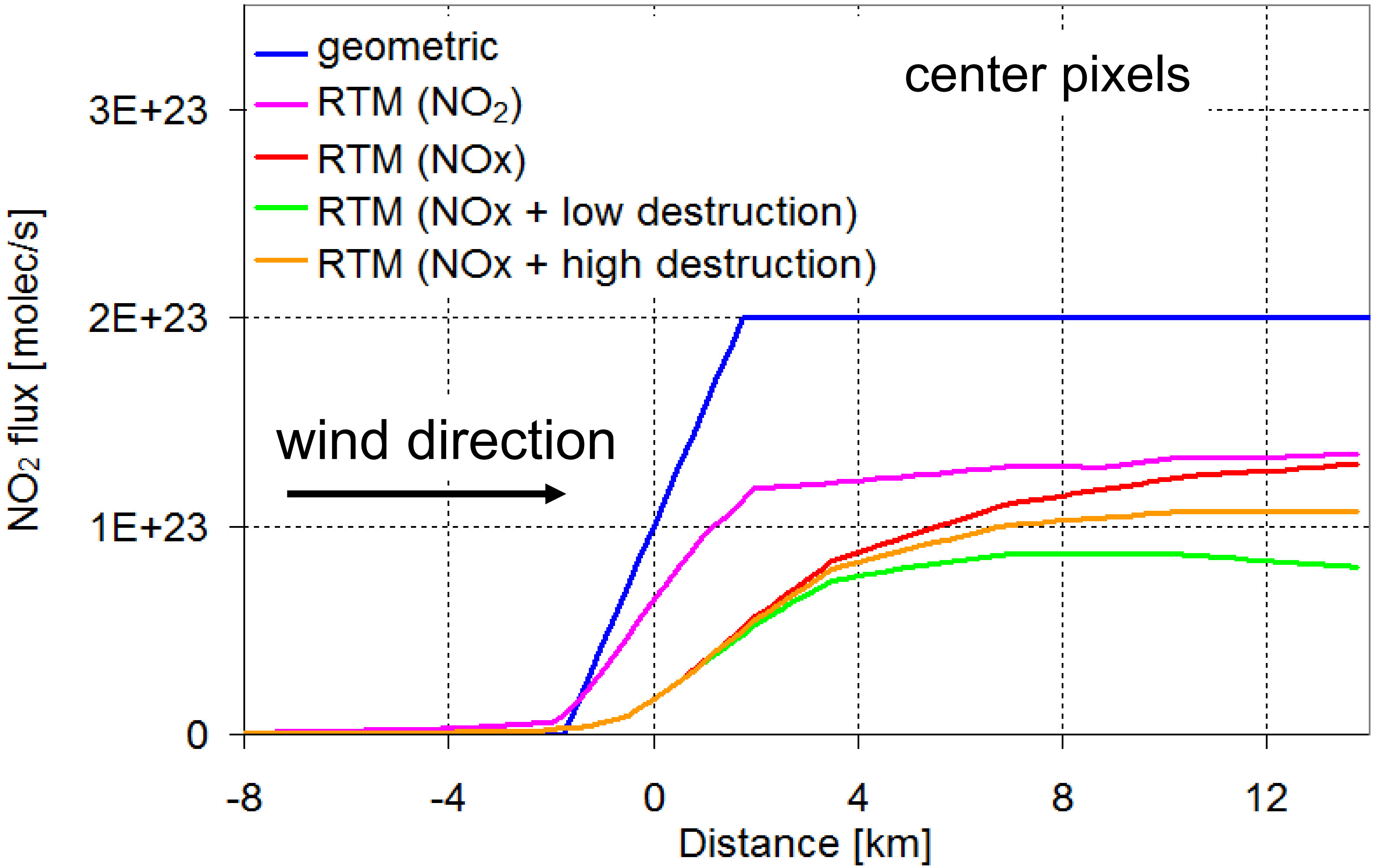
From wind fields and the $NO_2$ VCDs the flux is calculated. The divergence of the flux yields the emissions (Beirle et al., Science Adv., 2019)



## B) Calculating the divergence of the flux

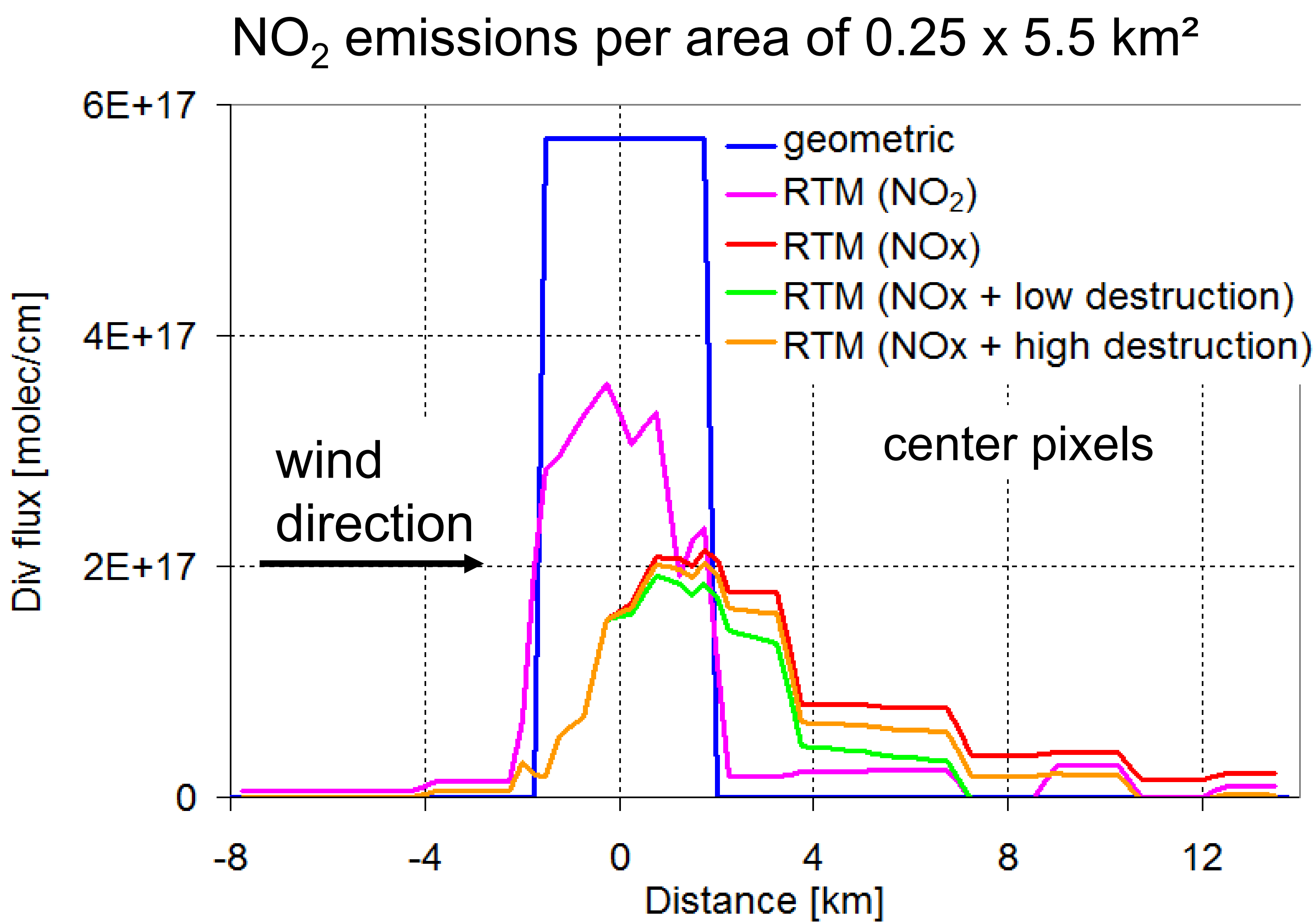
The flux is the product of the VCD, the wind speed and the across plume extension of the ground pixel:

$NO_2$ flux for standard scenario and wind speed of 1 m/s



## B) Calculating the divergence of the flux

The emissions are derived by the derivative against distance:



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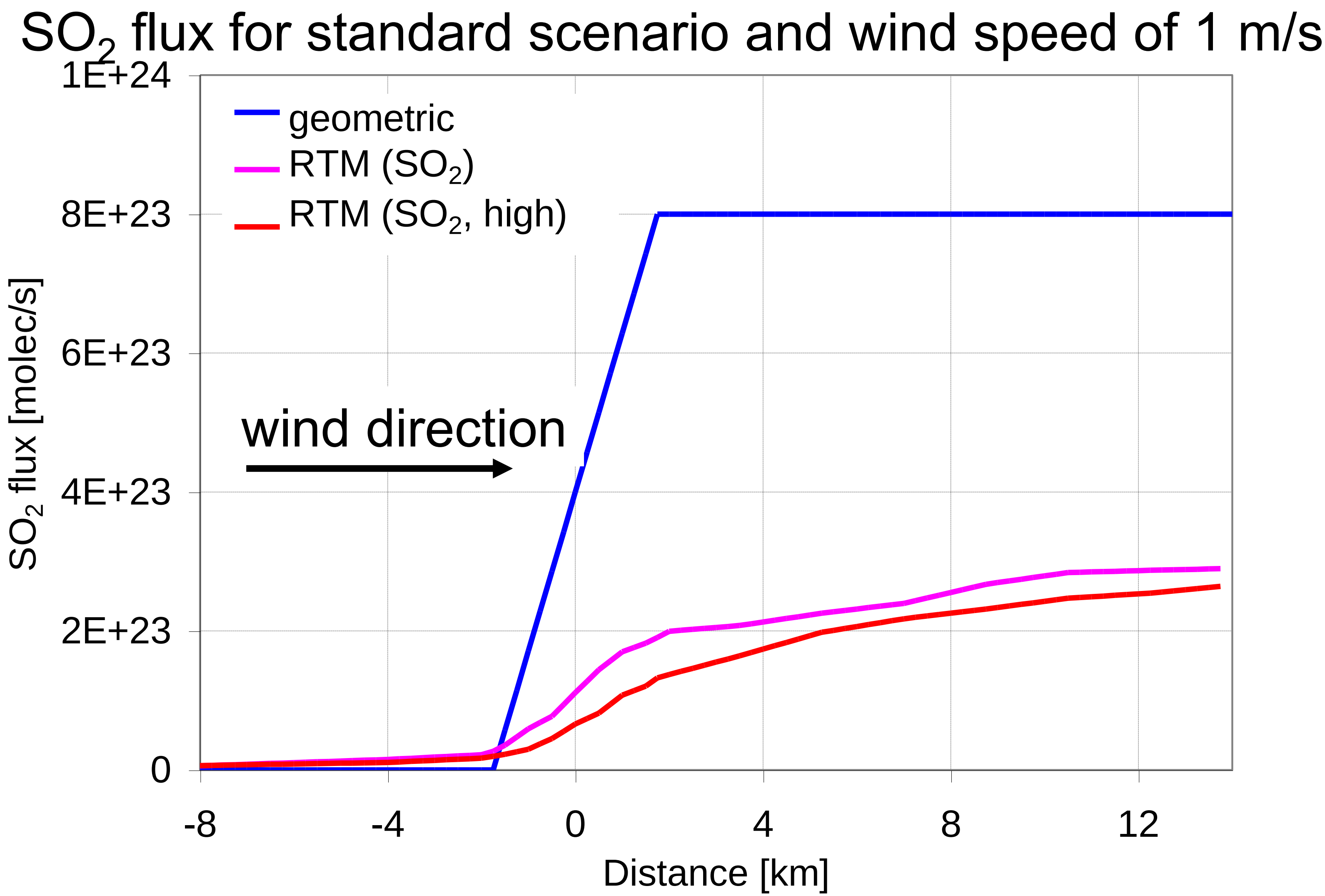

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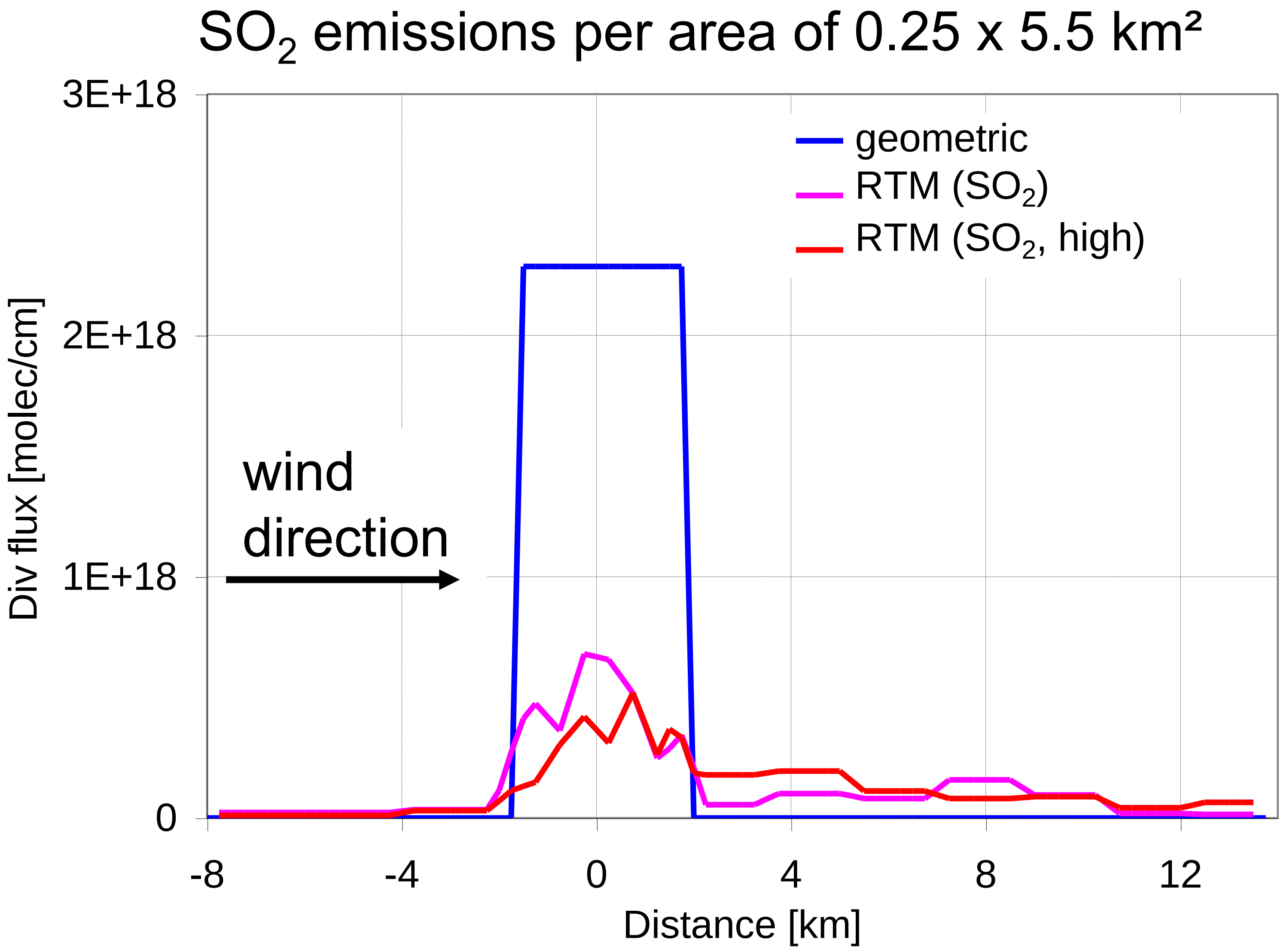
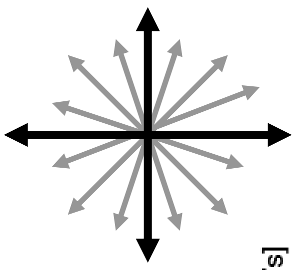


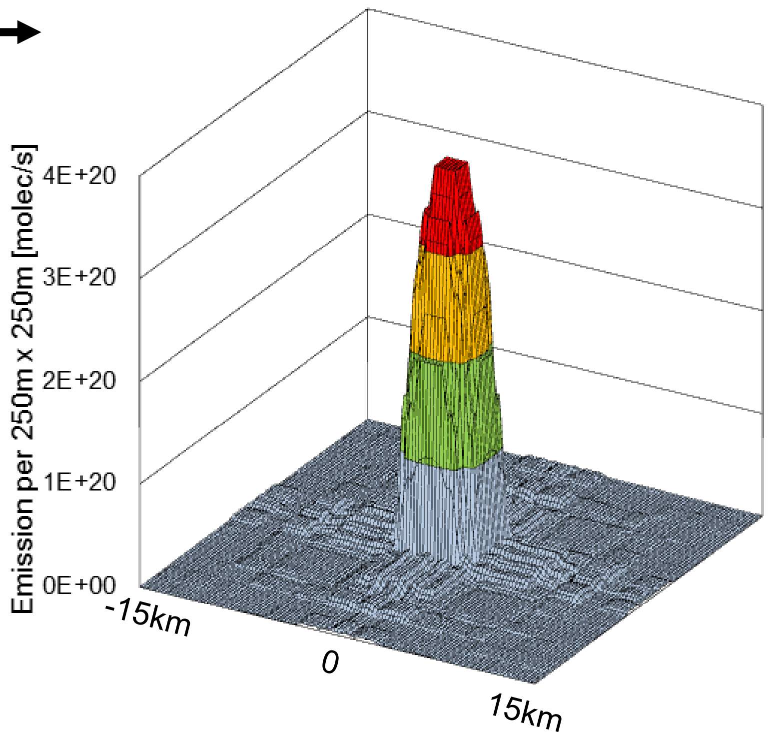
## Extension to 2 dimensions

4 directions are combined. This also considers the contribution of the across-plume pixels and should be representative for the real situation with any possible wind direction

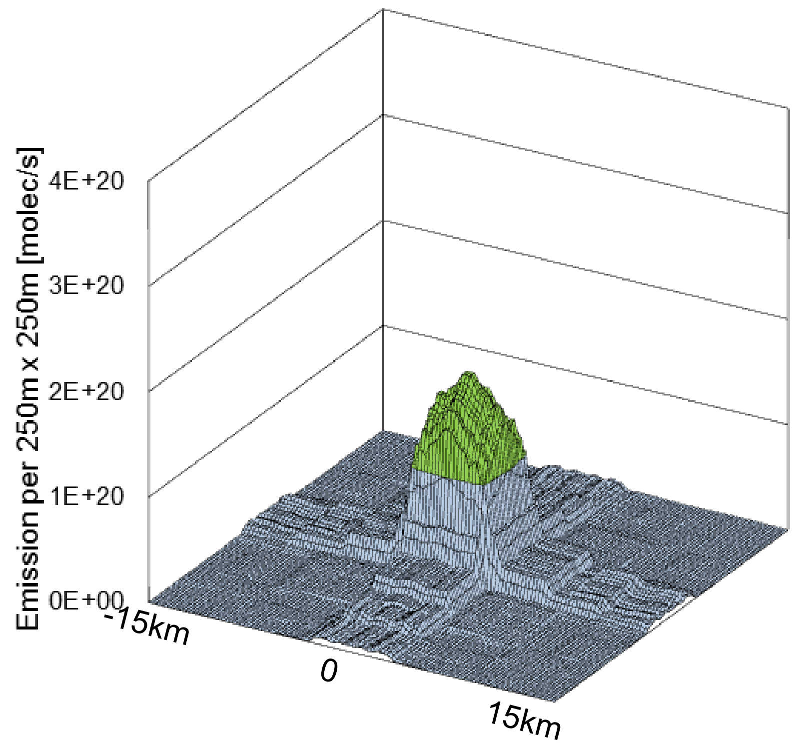
4 wind directions



only $NO_2$ emitted:
detected fraction: 68 (75)%
effective radius: 2.44 km




only NO emitted:
detected fraction: 56 (73)%
effective radius: 3.12 km



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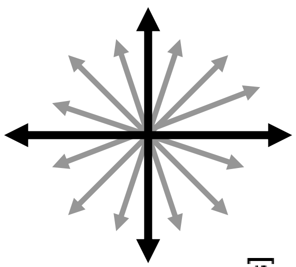
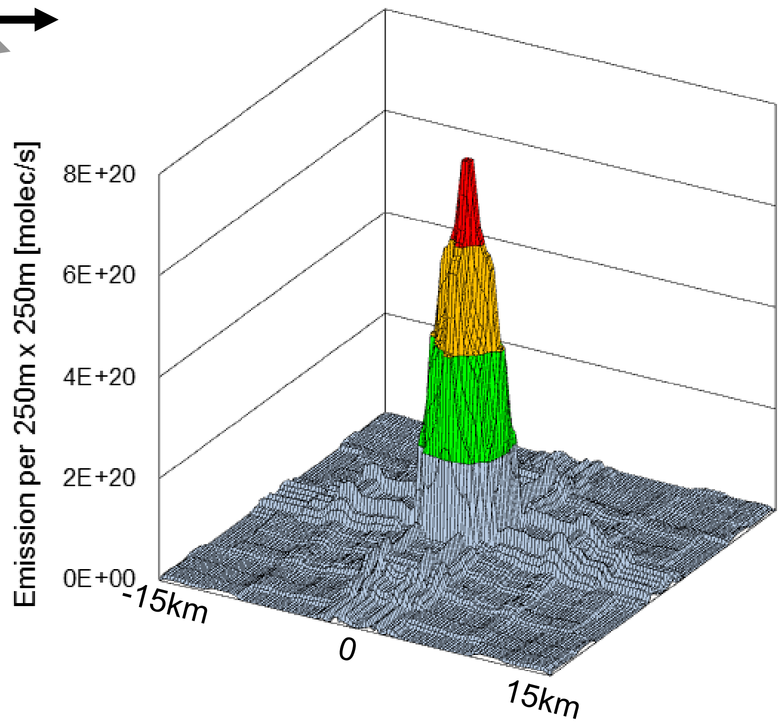
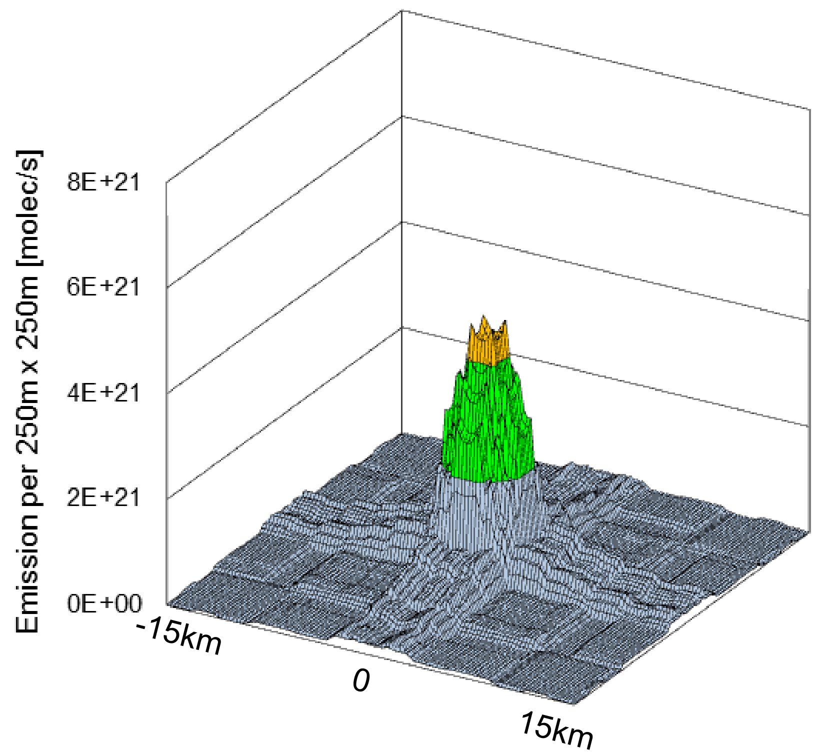


$SO_2$ low:
detected fraction: 24 (49)%
effective radius: 1.96 km




$SO_2$ high:
detected fraction: 20 (46)%
effective radius: 2.22 km



# Conclusions

- plumes from point sources are complex 3D structures, so far RTM in satellite retrievals does not account for this complexity

- there are two main effects:
    - horizontal light mixing
    - plume widening (increasing height)

- additional effects are:
    - NO to $NO_2$ conversion, $NO_x$ destruction
    - saturation for strong $SO_2$ emissions

- these effects cause typical underestimations:
    - $NO_2$: 25 – 40 %
    - $SO_2$: 55 – 80 %

- if 1D-AMF for 500 m layer would be applied:
    - $NO_2$: 10 – 30 %
    - $SO_2$: 52 – 80 %

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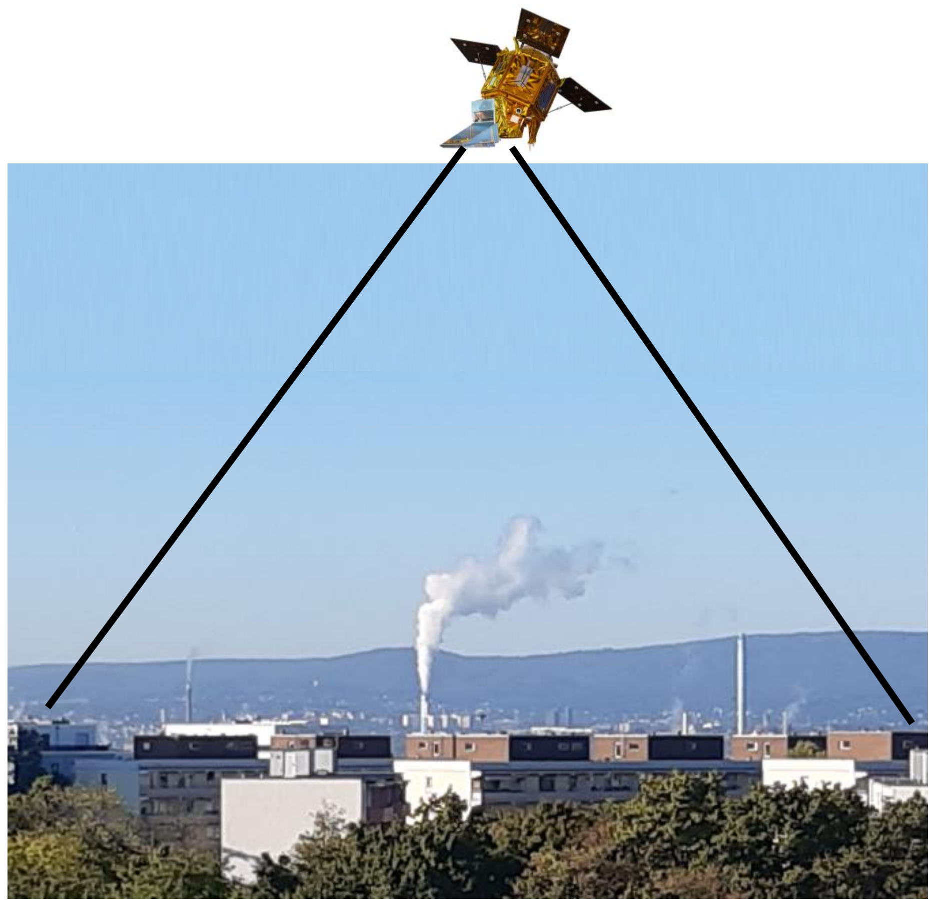

**Two additional effects are important and will also be considered in this study:**

**$NO_2$:**
The conversion of NO to $NO_2$ along the plume direction
(also destruction of $NO_x$ along the plume direction)

**$SO_2$:**
The very strong absorption in the early (narrow) plume for strong emissions

Because of these effects, the effect of the condensed plume close to the stack is usually not important.

# Results for different classes and aerosol scenarios