S1 Additional information

S1.1 MYSTIC NetCDF input file for the urban canopy

```
netcdf triangle_example {
    dimensions:
            Nvert = 6 ;
            Ndim = 3 ;
            Ntriangles = 5 ;
            Ncorner = 3 ;
            N_materials = 4 ;

    variables:
            double vertices(Nvert, Ndim) ;
                    vertices:_FillValue = NaN ;
            int64 triangles(Ntriangles, Ncorner) ;
            int64 material_of_triangle(Ntriangles) ;
            double material_albedo(N_materials) ;
                    material_albedo:_FillValue = NaN ;
            string material_type(N_materials) ;
            double temperature_of_triangle(Ntriangles) ;
                    temperature_of_triangle:_FillValue = NaN ;
    data:

     vertices =
            5.56999999994878, -6.07999999998719, 8.2,
            5.56999999994878, -6.07999999998719, 0,
            -3.09999999997672, 4.48000000001048, 8.2,
            -3.09999999997672, 4.48000000001048, 0,
            6.40000000002328, 12.320000000007, 8.2,
            6.40000000002328, 12.320000000007, 0;

     triangles =
            0, 2, 5,
            0, 2, 1,
            1, 2, 3,
            2, 4, 5,
            2, 4, 3,

     material_of_triangle = 0, 1, 1, 0, 1;

     material_albedo = 0.1, 0.1;

     material_type = "roof", "wall";

     temperature_of_triangle = 273.15, 273.15, 273.15, 273.15, 273.15;
}
```

The MYSTIC NetCDF input files for the urban canopy contains a temperature for each triangles, which is not used in the radiative transfer calculations for this study, but needs to be set for avoiding a error message from the model.

S1.2 MYSTIC input tables

Table S1. MYSTIC input for AMFs computation.

Parameter	Value
Number of photons	50000 or 500000
Wavelength [nm]	490
Solar zenith angle [°]	60 or 30
Solar azimuth angle [°]	0, 90
Viewing zenith angle [°]	0.24 - 5.47
Viewing azimuth angle [°]	90, 270
Surface albedo	0.1 or 0.2
Aircraft position x [m]	600
Aircraft position y [m]	2.5 - 997.5
Aircraft position z [m]	6000
Simulation resolution [m]	5 and 50
Simulation domain [boxes]	20×20×41
Horizontal resolution [m]	5 and 50
Vertical resolution (0 - 45m) [m]	5
Vertical resolution (50 - 1000m) [m]	100
Vertical resolution (1000 - 1500m) [m]	250
Vertical resolution (2000 - 21000m) [m]	1000
Aerosol absorption and scattering	off

S1.3 3D NO_2 concentration field

To obtain a realistic synthetic 3D NO_2 concentration field, we proceeded as following:

- We summed emissions from cars, busses, trucks and motorbikes from the road emission inventories from the city of Zurich (2015)
- We rasterized the emission field to a 5 m x 5 m resolution grid and divided each grid cell by the maximum grid cell value.
- We multiplied the obtained 2D field with an immission value of 110 [$\mu g\ m^{-3}$] and added a background of 15[$\mu g\ m^{-3}$], which are respectively typical high and background values found at measurement stations close to the road and on a background site (e.g. https://www.stadt-zuerich.ch/gud/de/index/umwelt_energie/luftqualitaet/messdaten/verlauf-24-stunden.html). Finally, we smoothed the concentration field with a Gaussian filter with a standard deviation of 5 m to mimic the effect of turbulent dispersion.
- From the obtained ground concentration map we created 3D concentrations applying the following function to every ground pixel. Between $h_0 = 0$ m and $h_1 = 100$ m a linear concentration decrease with altitude was applied with the level corresponding concentrations c_0 = ground concentration (grid cell concentration) and c_1 = 1/5 of the ground concentration over a background pixel. From h_1 upwards, an exponential decay function (A exp(t z) + y0) with A = 1.6, t = -1.39 and y0 = 0.09 parameters was applied. This parameters were defined by fitting a function to a measured NO_2 profile from the MuNIC campaign.

– Finally the VCD calculated using the created 3D NO_2 concentration field was compared with NO_2 VCDs from the MuNIC measurement campaign (2016).

S2 Additional Figures

S2.1 $\mathbf{NO_2}$ maps obtained from APEX and GRAMM/GRAL (preliminary results)

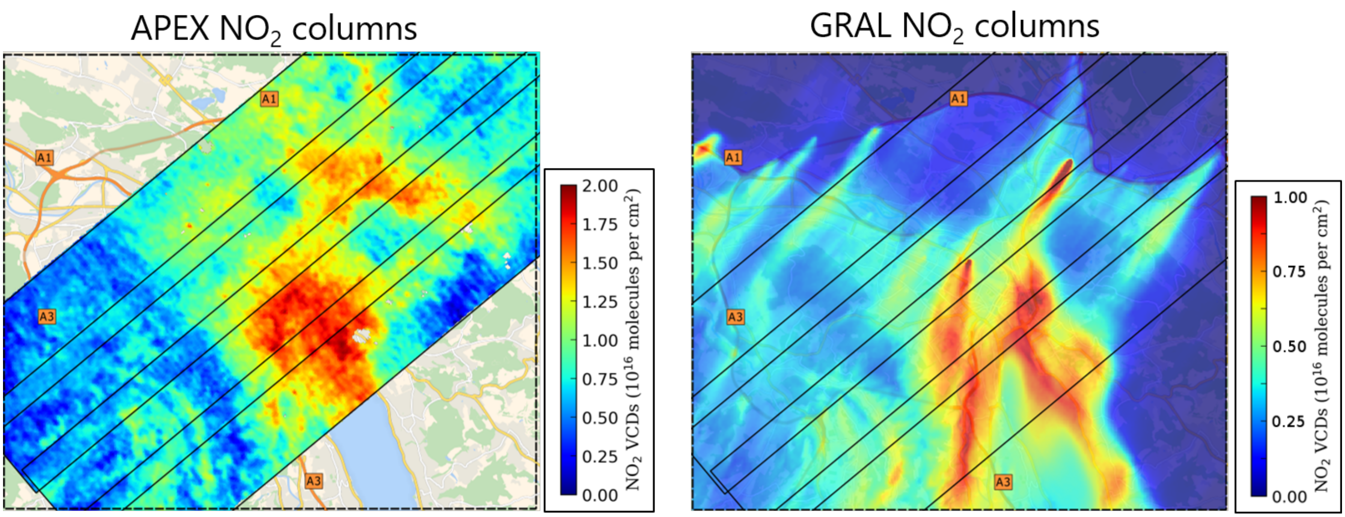

Figure S1. NO_2 columns retrieved from APEX imaging spectrometer and from city-scale GRAMM/GRAL modelling system (preliminary results shown by Kuhlmann et al., 2017).

S2.2 SCDs for a solar zenith angle of 30°

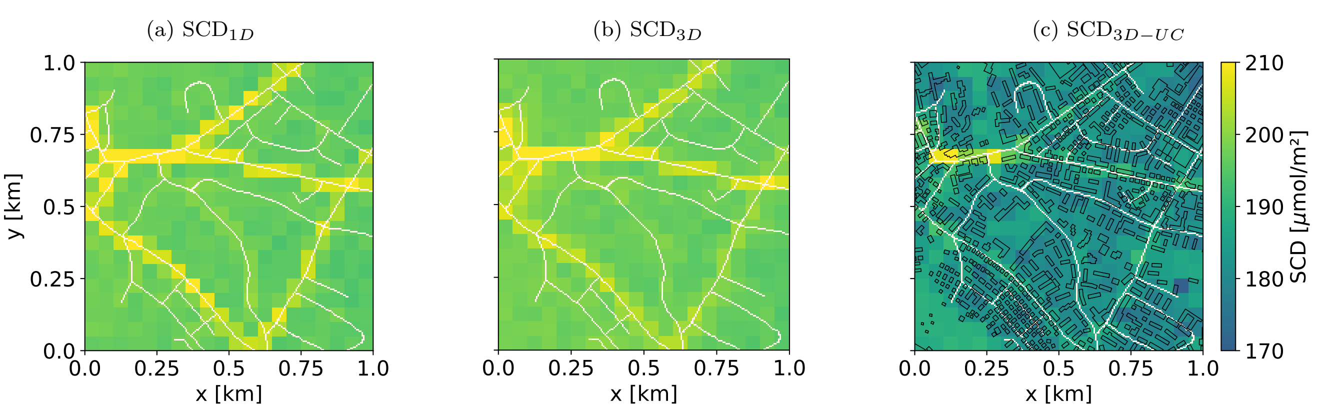

Figure S2. SCDs for a simulation with SZA of 30° with 1D-layer AMFs simulation (a), 3D-box AMFs without (b) and with (c) buildings. The roads are drown in white and the building contours in black for the simulation with buildings.

S2.3 Difference plot for SCDs for a solar zenith angle of 30°

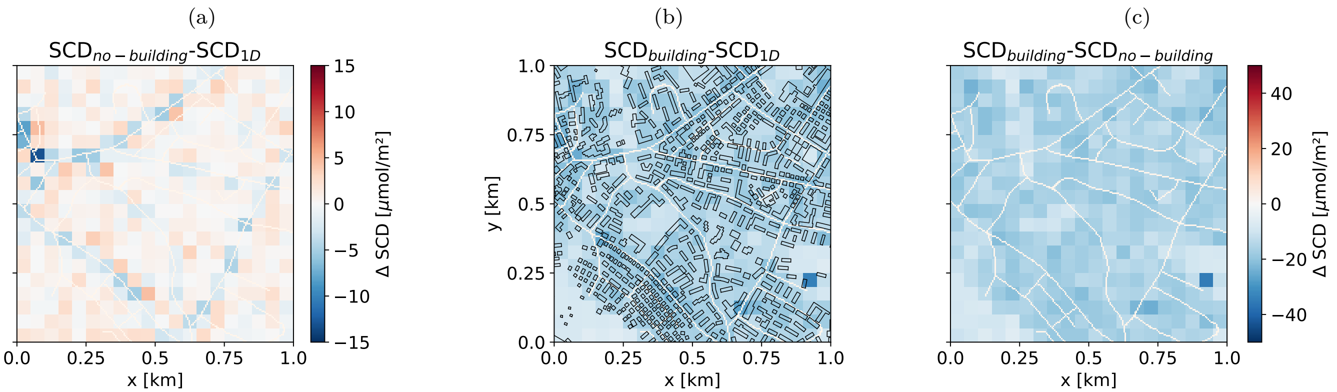

Figure S3. Difference plots for SCDs calculated with a solar zenith angle of 30°. (a) Difference plot between SCDs calculates with 3D-box AMFs and the SCDs calculated with 1D-layer AMFs. (b) Difference plot between SCDs calculated with 3D-box AMFs including the urban canopy and SCDs calculated with 1D-layer AMFs. (c) Difference plot between SCDs calculated with 3D-box AMFs with and without including the urban canopy.

S2.4 Increased roof albedo for the high resolution scenario

Here we show the impact of an increased albedo on the building roofs. We changes the albedo of the roofs from 0.1 to 0.2. We observe the increase of AMFs and therefore SCDs above the buildings because more photons are scattered on the roof with a higher albedo, compared to the lower ground albedo.

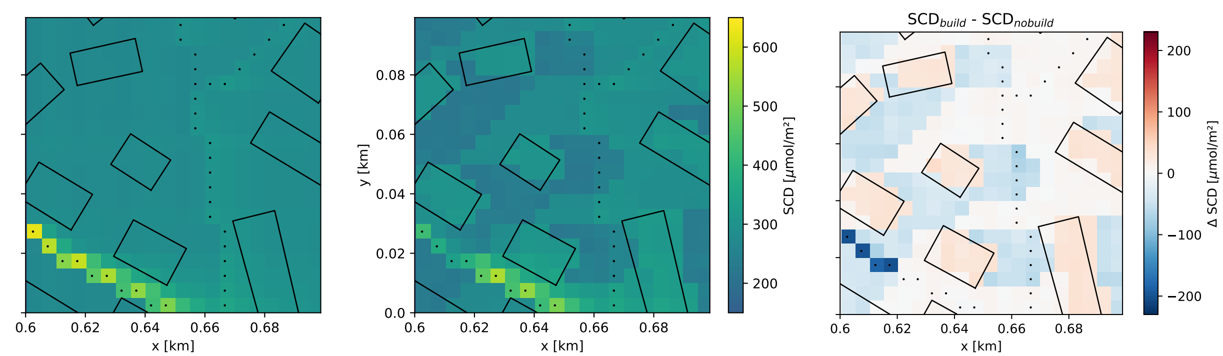

Figure S4. SCDs for a SAA of 90° for 3D-box AMFs simulation without (a) and with (b) buildings and the difference between both (c). The roof albedo was set at 0.2. The roads are drawn in white and the building contours in black for the simulation with buildings

S2.5 SCDs for a SAA=270°

We also computed SCDs with the 3D box-AMFs module for a SAA=270° (see Fig. S5). Similarly to observations made in the paper, SCD are smeared mostly in the direction of the main optical path (E-W-direction).

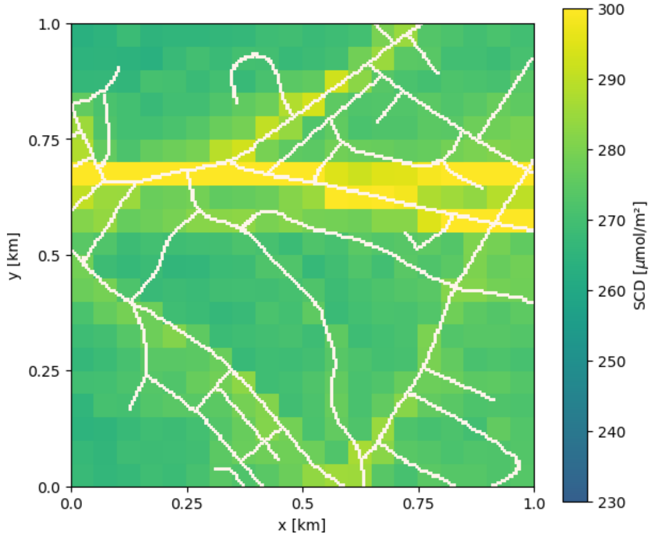

Figure S5. SCD without UC and a solar azimuth angle of 270°

S2.6 Footprints

S2.6.1 Footprints with aerosols

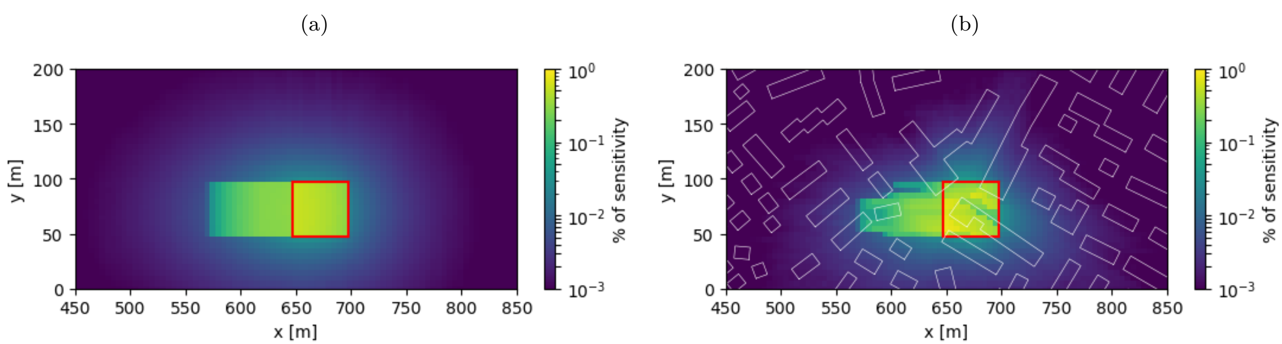

Figure S6. (a) Footprint without buildings and with aerosols. 55.2% of the signal is located outside the ground pixel (i.e. outside the red frame). (b) Footprint with buildings and aerosols. 55.2% of the instrument sensitivity is located outside the ground pixel. Building contours in white.

S2.6.2 Footprints for SZA=20° and SZA=40°

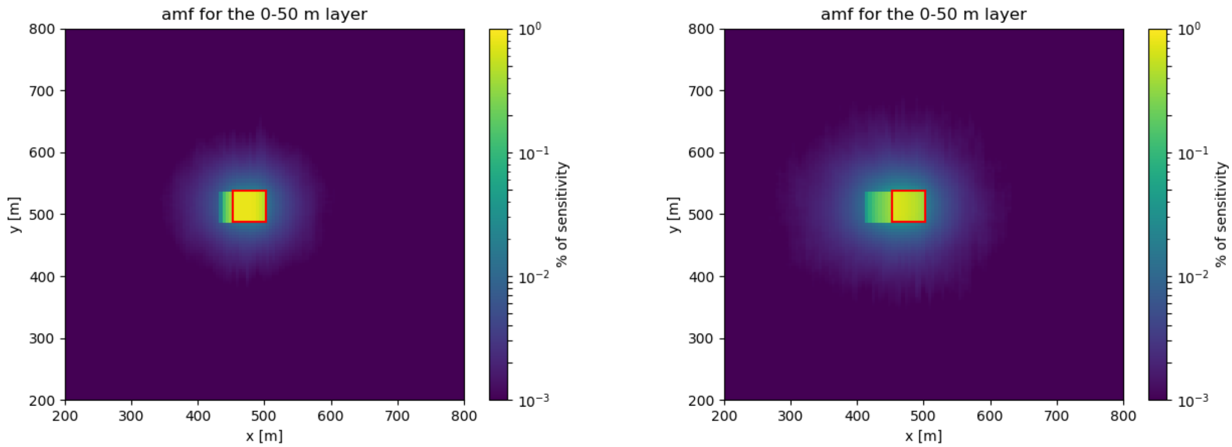

Figure S7. Effect of SZA on APEX footprint. Simulation with SZA = 20° and 40°. Respectively 27.4 and 45.2 % of the sensitivity is located outside the ground pixel (red square)

S3 Computational time

S3.1 Simulations with buildings

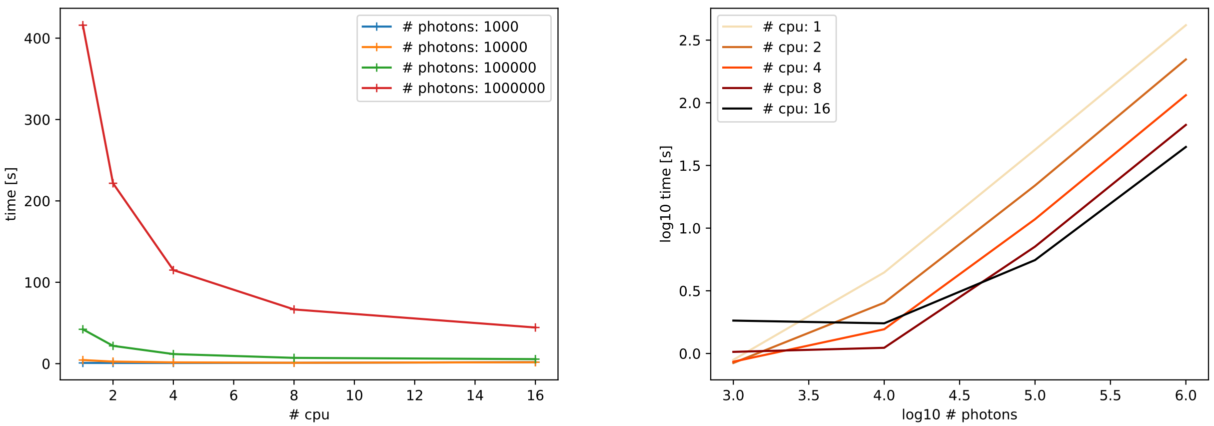

Figure S8. Computational time for simulations with buildings for (left) number of used CPUs and (right) number of photon.

S3.2 Simulations without buildings

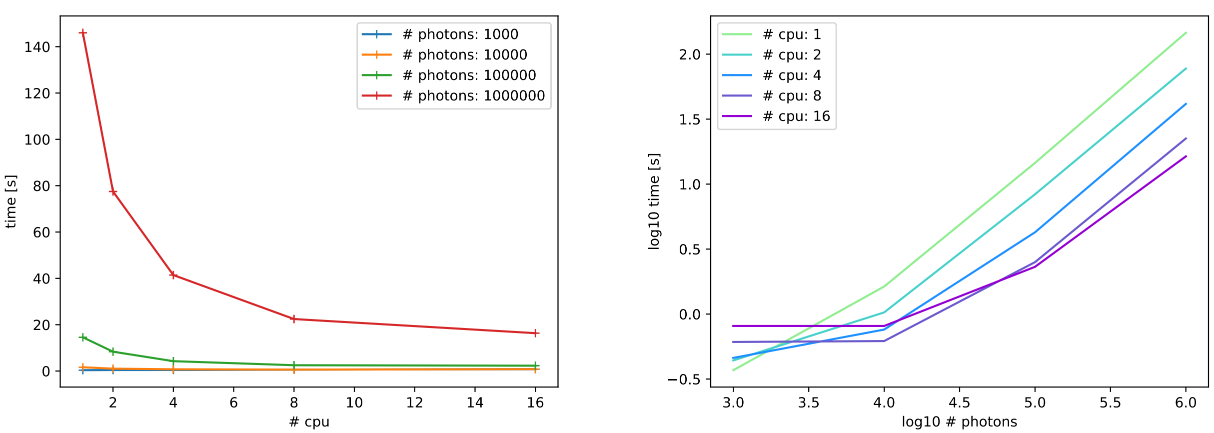

Figure S9. Computational time for photon amount, without buildings and different number of CPUs.

References

Kuhlmann, G., Berchet, A., and Brunner, D.: High-resolution remote sensing and modelling of NO2 air pollution over the city of Zurich, in: 10th EARSeL SIG Imaging Spectroscopy Workshop 2017, Zurich, Switzerland, 2017.