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Photochemistry Study with the Urban Microscale Model PALM-4U using the CBM-IV Mechanism

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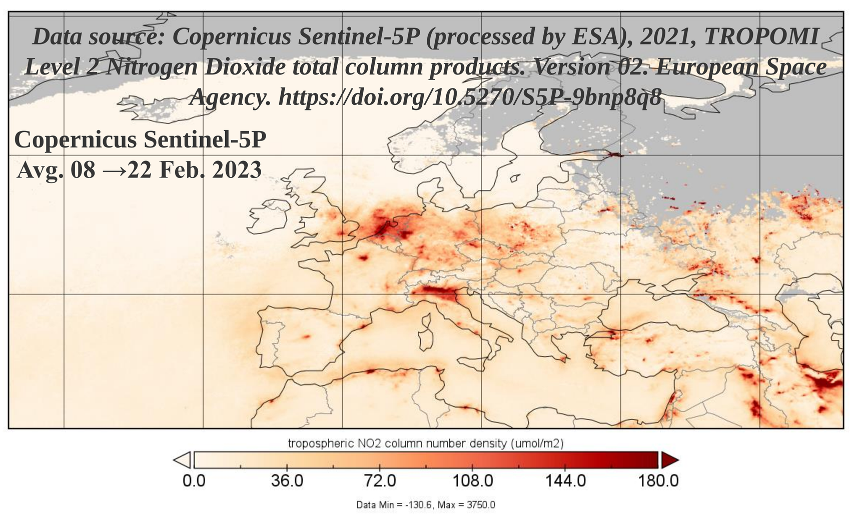
Urban air quality

Fig.1= The tropospheric NO_2 column number density (data: Copernicus Sentinel-5P satellite) is shown for Europe. Large levels of NO_2 over the urban regions are distinctively present.



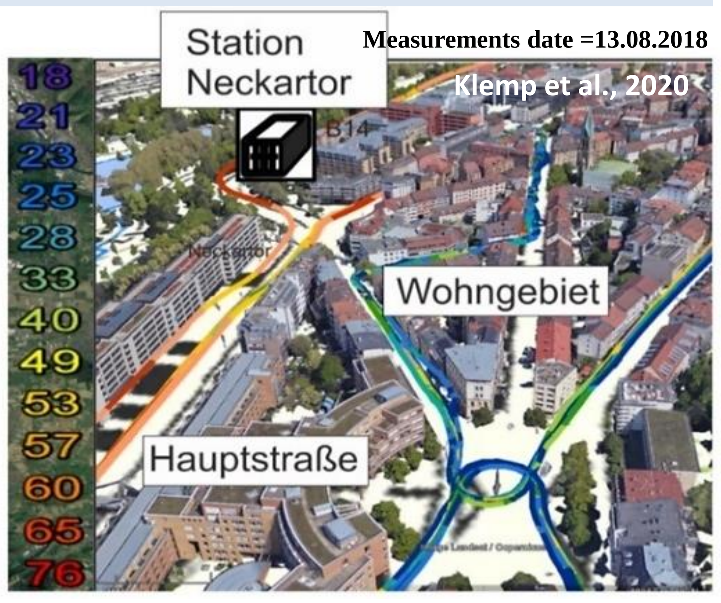


Fig. 2 = Large scale variability has been shown by measurements (via MobiLab) of NO_2 (in ppb) in the city of Stuttgart.

PALM-4U boundary conditions and CBM-IV based simulation

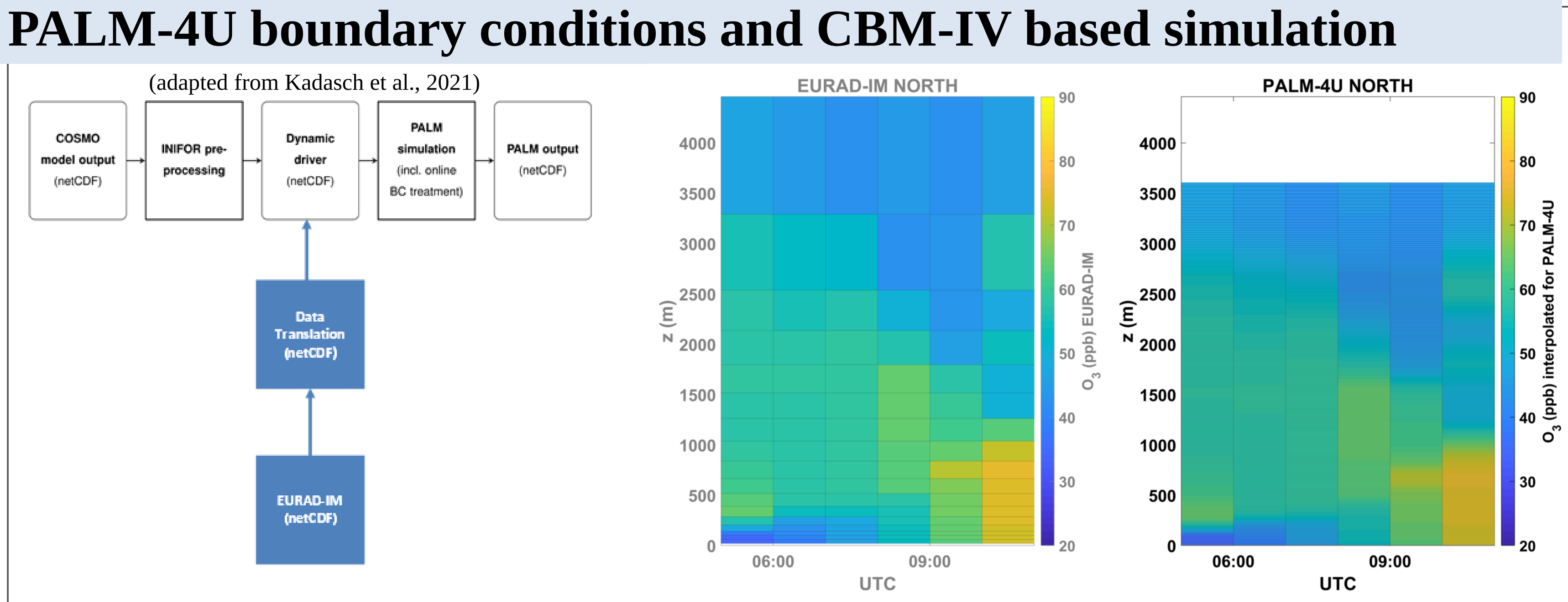


Fig. 5: The LHS shows an existing transfer path for the meteorological components (Kadasch et al., 2021) to drive PALM-4U boundary conditions. Also, the new transfer path is realised by us for the chemical components from the results of EURAD-IM (Elbern et al., 2007). The RHS shows an example of the extensive transfer of the ozone concentration from EURAD-IM, which varies in altitude and time of day, shown on the northern boundary surface of the PALM-4U model (typically 10 m resolution).

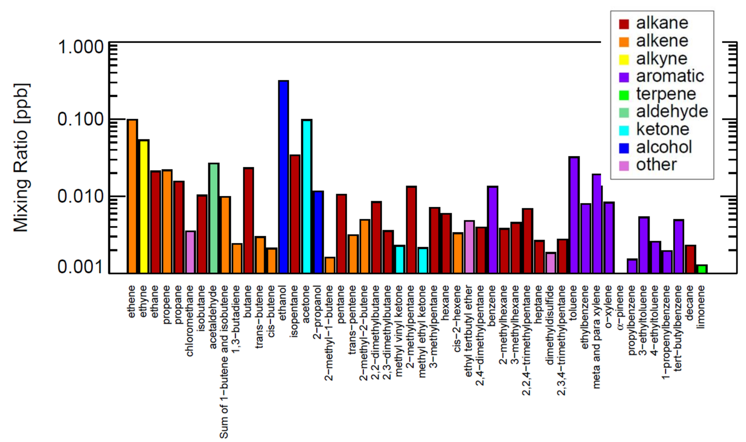


Fig. 6: The measured traffic-related VOCs/NO_x ratios are used to quantify the VOCs emissions in PALM-4U. The mean VOCs pattern in the Heslacher Tunnel is shown for the summer of 2017/2018. The VOCs data is the average of five tunnel measurements via MobiLab.

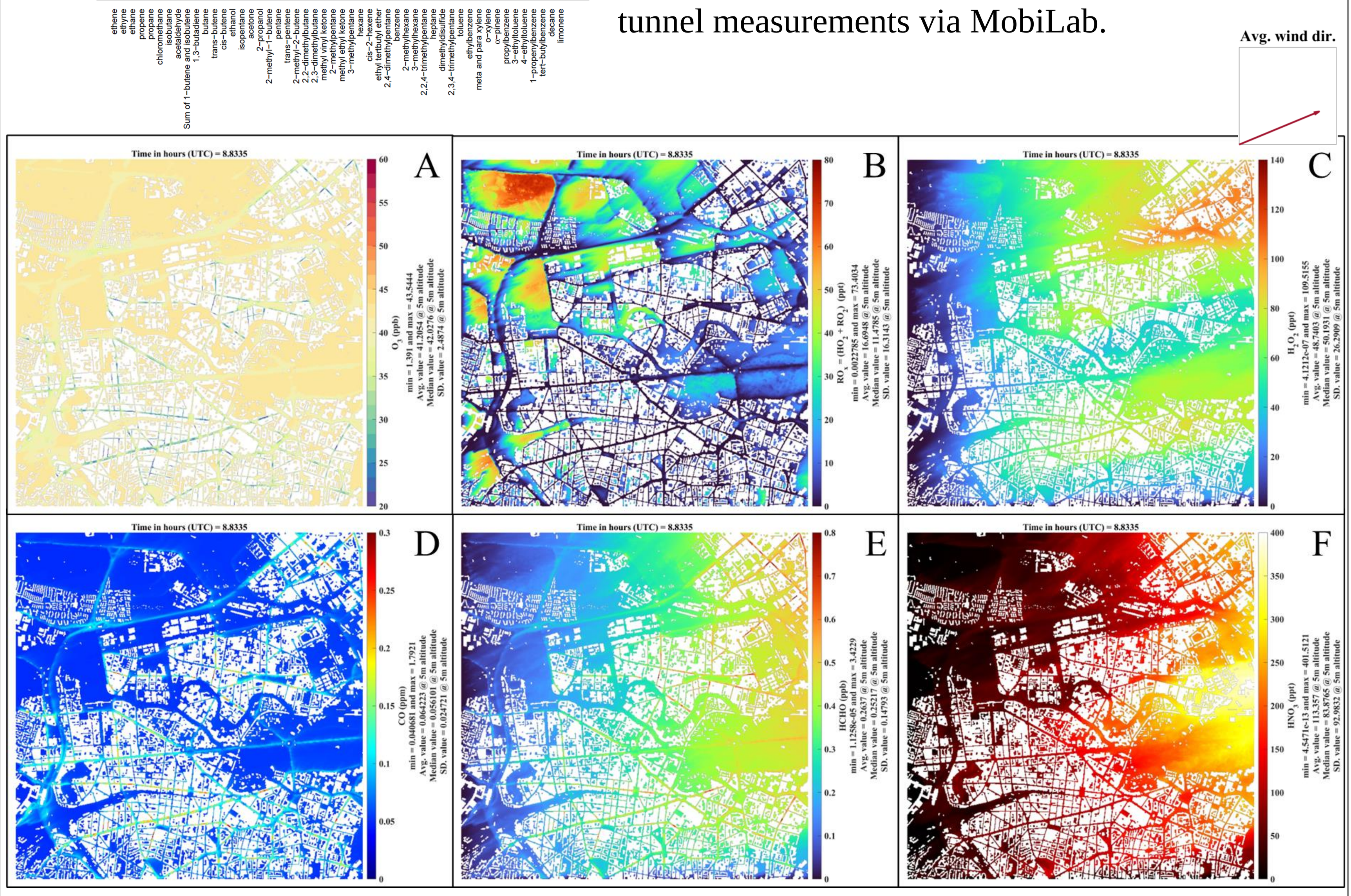


Fig. 7: The CBM-IV based simulation represents an area of 6.72×6.72 km^2 around the Ernst-Reuter-Platz in Berlin . The spatial distribution of concentrations of simulated radical-related species are shown for the time 8.8UTC on 26 June 2019. The white spaces in the domain represent buildings/structures. Subplots: A= O_3 (ppb), B= RO_x (ppt), C= H_2O_2 (ppt), D= CO (ppm) , E= HCHO (ppb), F= HNO_3 (ppt)

- Relatively lower concentrations of O_3 can be seen on the streets/roads (Fig.7, A). This is mainly happened due to the titration of O_3 (background EURAD-IM) with traffic-linked high NO concentrations (internal PALM-4U emissions). Enhanced concentrations of RO_x (Fig.7, B) over the vegetation (no traffic areas) indicate radical photochemistry under lower NO_x conditions is dominant and could potentially lead to O_3 formation.

CBM-IV vs MCM-3.3.1 (Box model based comparison)

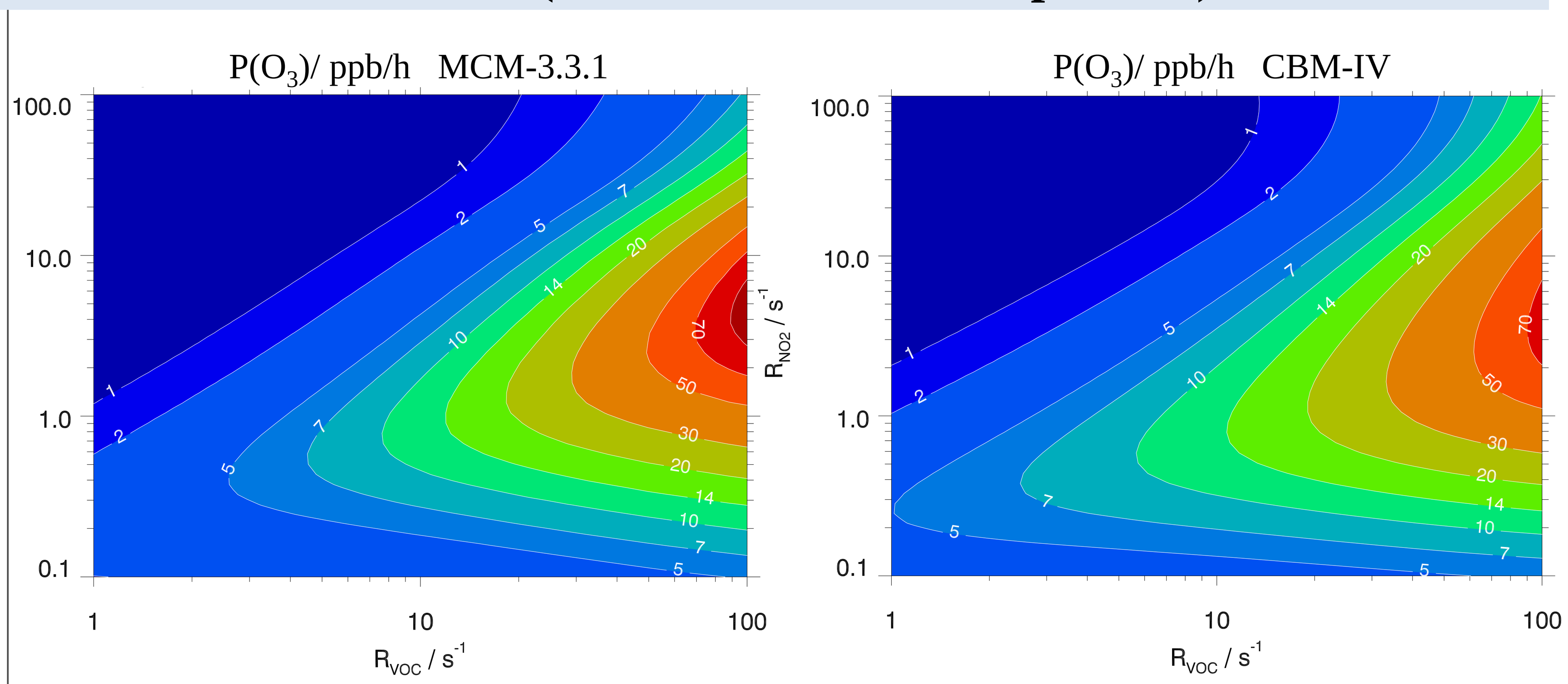


Fig. 3: The local O_3 production rates [P(O_3)] in ppb h^{-1} are shown as a function of VOC and NO_2 expressed by their reactivity (versus OH radical) R_{VOC} (x-axis) and R_{NO2} (y-axis), respectively. The RHS and LHS plots are based on Master Chemical Mechanism (MCM)-3.3.1 (Saunders et al., 2003) and Carbon Bond Mechanism (CBM)-IV (Gery et al., 1989), respectively. General conditions : Latitude: 52.5° northern latitude, radiation conditions: 21. 06, local noon 12:00. The MCM-3.3.1 is based on roughly >10^4 reactions (>10^3 species) while CBM-IV is based on only <100 reactions (<50 species).

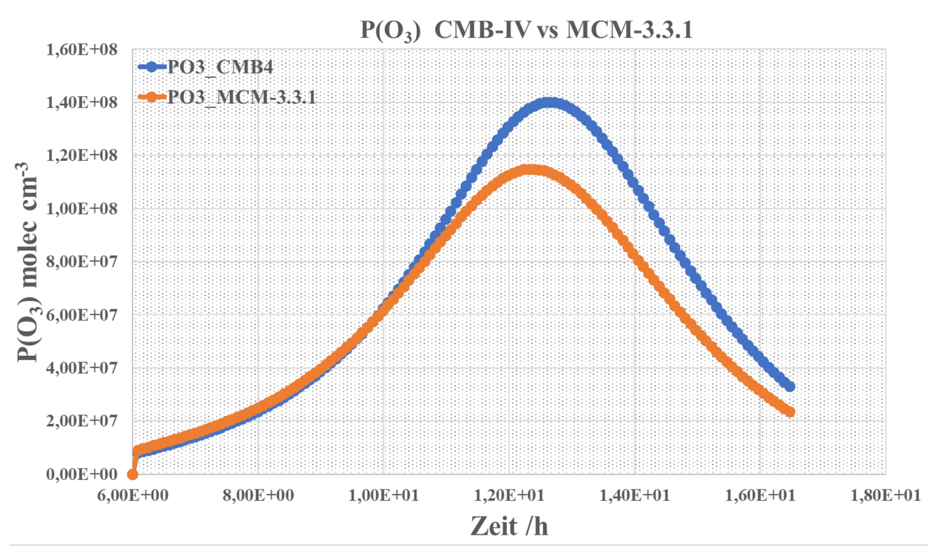


Fig. 4: Time series of P(O_3) is shown for both mechanisms. The starting conditions (R_{VOC} = 10.1s^{-1} and R_{NO2} = 17.6s^{-1}) correspond to the summer inner city mean results found in Berlin during 2017-2018. The comparison in terms of cumulative P(O_3) has shown a difference of only about 20% with higher values calculated by CBM-IV.

- The analysis (box model based) between MCM-3.3.1 and CBM-IV has shown that there are small differences (about 20 %) between the two mechanisms in terms of describing the production of ozone in typical urban conditions. Nevertheless, the use of a relatively less detailed CBM-IV mechanism in PALM-4U would be less computationally expensive/ demanding to study the production of ozone in urban regions.

Building's shadow impact on photolysis frequencies in PALM-4U

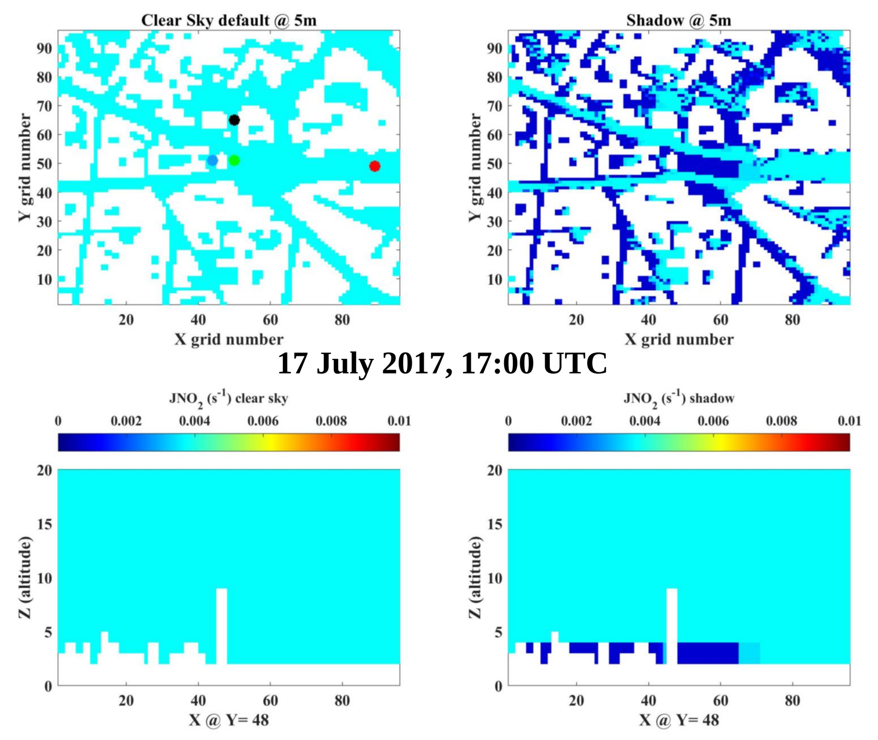


Fig. 9: Ratios (shadows / clear sky) for NO and NO_2 have shown for different grids at 5m (same colors: Fig. 8, top left) altitude in the model domain.

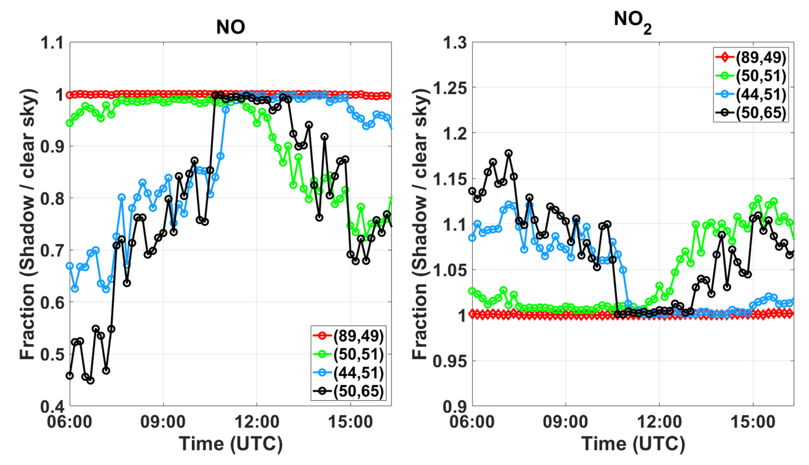


Fig. 8: The simulated JNO_2 is shown for a domain (960×960×185 m^3) around the Ernst-Reuter-Platz (Berlin). The left column shows the default (clear sky) mode of the model. The right column presents JNO_2 with shadow's approximation. The approx. is based on the zenith angle with 80% reduction for photolysis at ≤25m altitude.

- Significant impact of shadows on the photochemistry has seen in the small street canyons and residential areas. A future consideration of building's shadows will be essential to reflect the true street canyon photochemistry.

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[UC]² Urban Climate Under Change
Stadtklima im Wandel