T3.1. Characterization of urban dispersion using advanced observations-based methodologies and modelling

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Inv.: CEREA/CNRS, KNMI, FMI

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Main scope of Task 3.1

- Improve urban aerosol particle emissions combining in-situ measurements (long-term, near-real time, source apportionment) and novel modelling tools (Large-Eddy Simulation LES, data assimilation, bottom-up emission models, air quality and dispersion modelling)
- Main thematic activities:
  - Helsinki: Combination of aerosol particle fluxes and PArallelized LES Model (PALM) to quantify urban emission fluxes
  - Paris: Use of MUNICH model to simulate dispersion and formation of particles
  - Turku: SILAM and PALM interfaced to simulate passive-tracer plume
  - Barcelona: Constraining BC/UFP emissions at the road-link level combining observations and the CALIOPE-Urban dispersion modelling tool
  - Rotterdam: Dutch Atmospheric Large Eddy Simulation (DALES) implementation of Rotterdam urban canopy

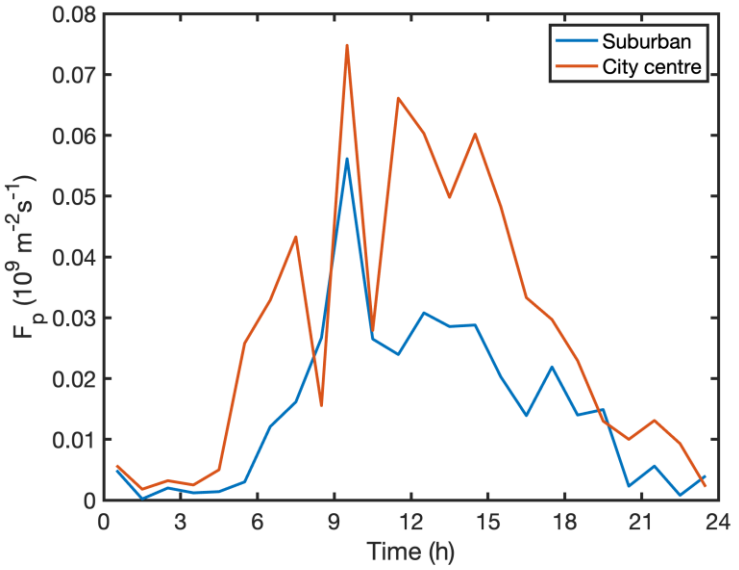
Novel improvement of pollutant emission data products

Aerosol particle fluxes and large eddy simulation (LES) combined to quantify the spatial and temporal dynamics of urban emission fluxes

Technique developed in Helsinki and tested in Paris (ICOScities observations)

Status: LES simulation setup planning ongoing

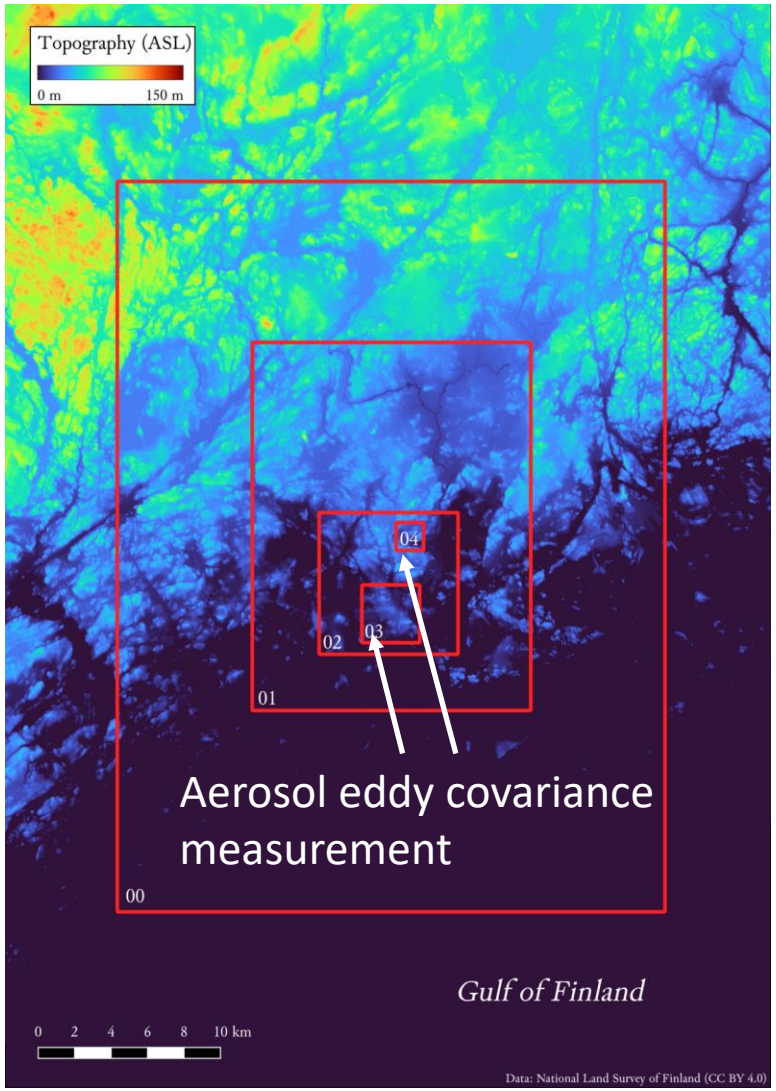
Diurnal variability of aerosol particle number flux in May 2022



Methods

Eddy covariance measurements + LES model PALM

Helsinki LES setup



Courtesy of Sasu Karttunen

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European Commission

HORIZON 2020

HELSINGIN YLIOPISTO

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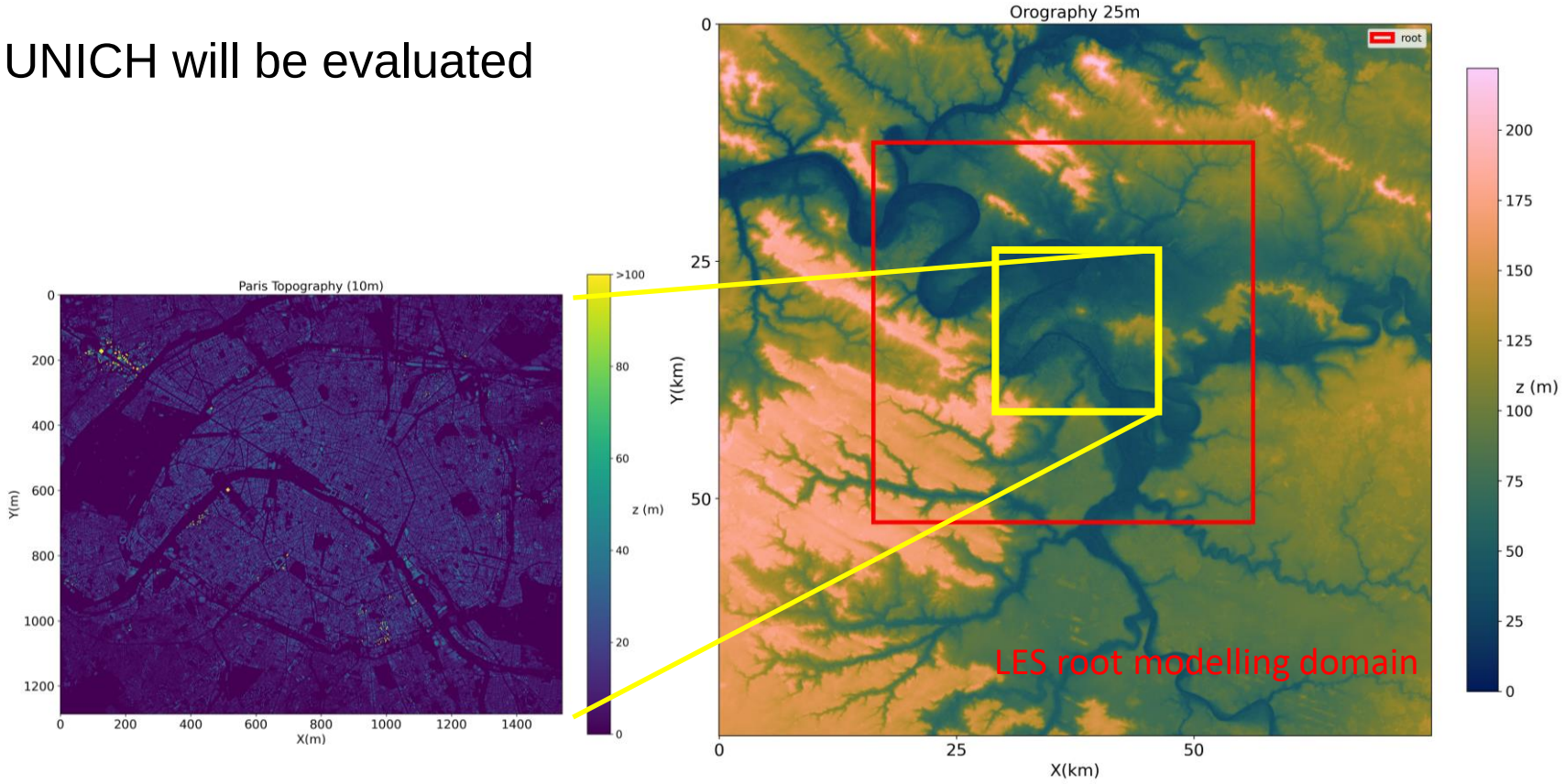
Paris boundary layer simulated using PALM and MUNICH

The street-network model MUNICH will be evaluated against PALM

Both used to simulate the dispersion processes between the urban surface and ABL and upscale

Status: LES simulation setup planning ongoing



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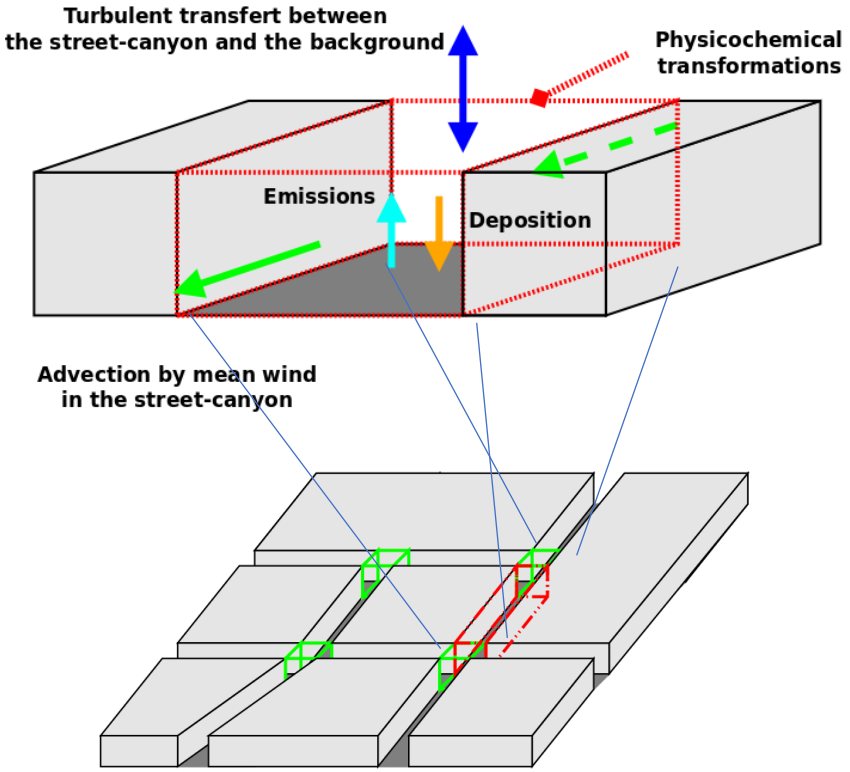
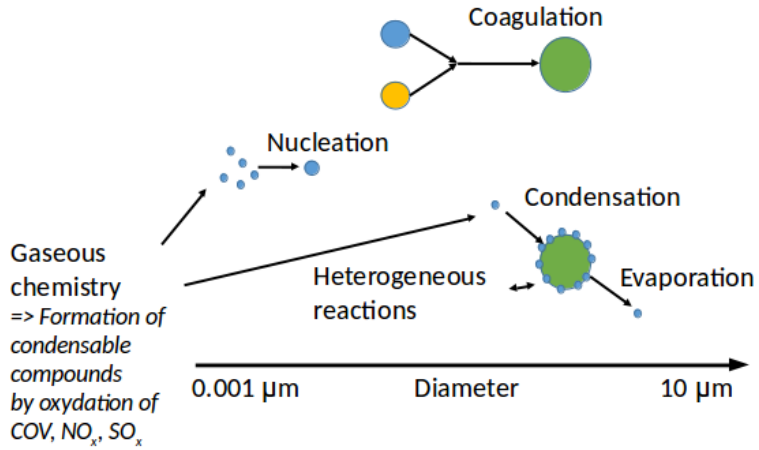
Street-scale modelling using the street-network model MUNICH

- Assumptions:
  - Concentrations are uniform in each street segment.
  - Width of the street and height of buildings are uniform.
  - Wind direction follows the street direction in the street
- Meteorology is parameterized



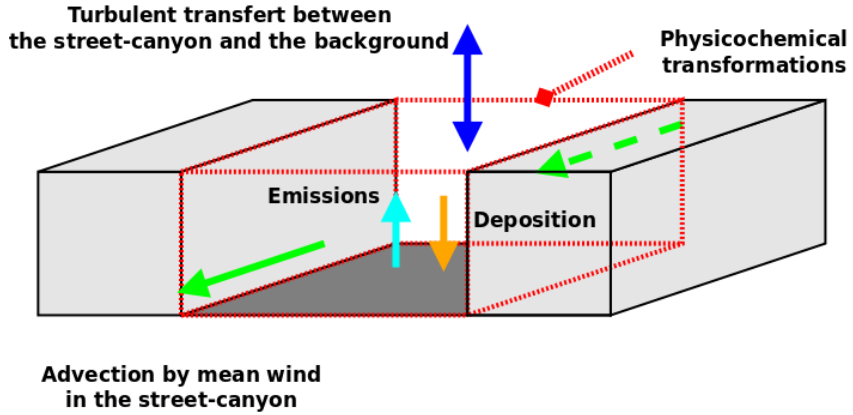
- Coupled to SSH-aerosol [Sartelet et al. 2020] to model the formation and ageing of gas and particles.

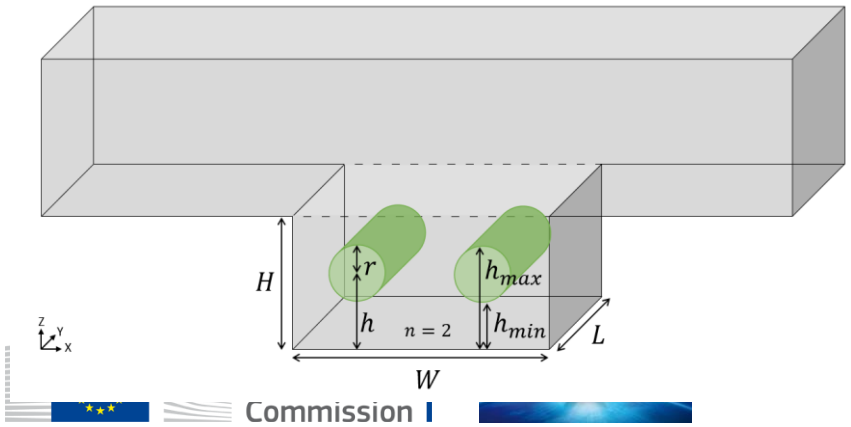


[Kim et al., 2018; Lugon et al. 2020; Kim et al. 2022]

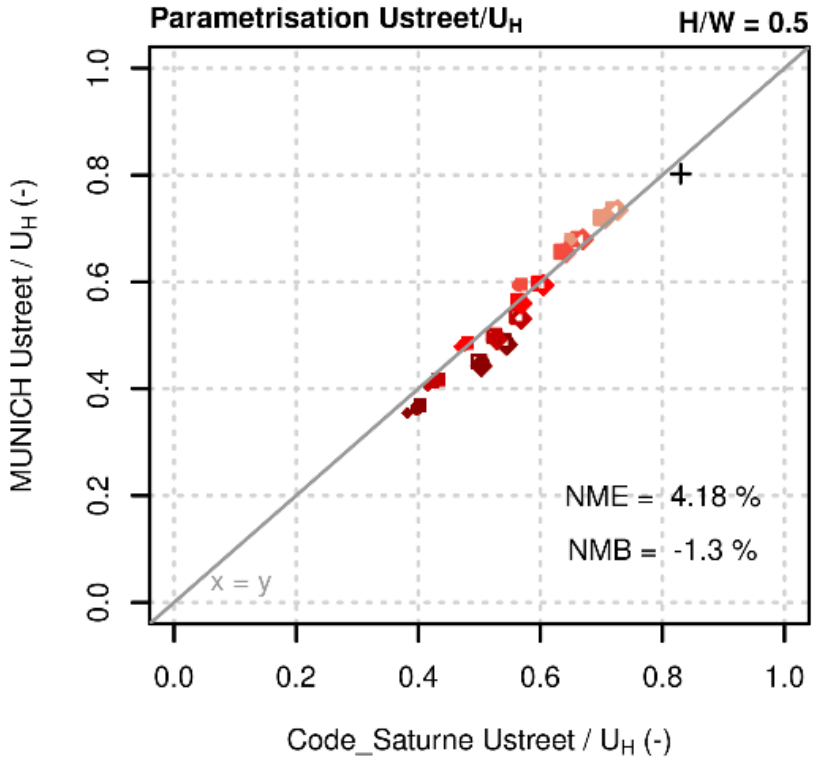
Free software available on Github https://github.com/cerea-lab/munich

Parameterizations in MUNICH



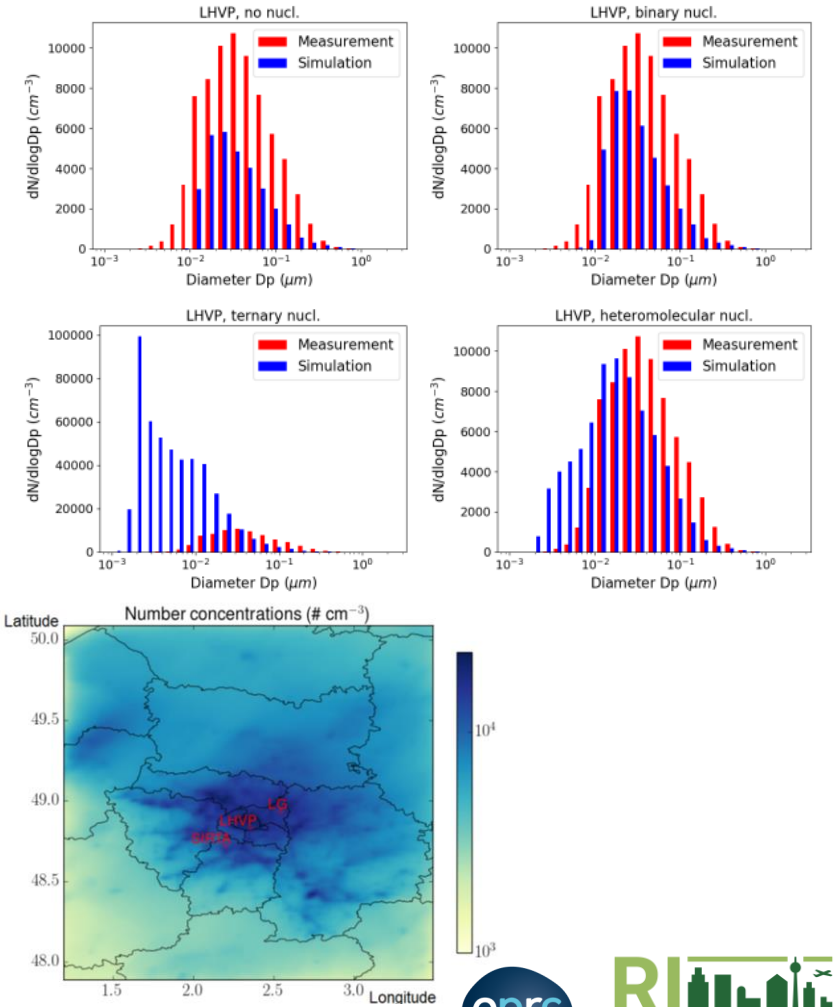


- Construction of parameterizations (turbulent transfer from the street to above; wind in the street) from the computational fluid dynamic tool Code_Saturne (k, ε) for case of **streets with trees** [Maison et al. 2022].
- **Objective in 3.1**: Further improve mass transfer parametrisations thanks to PALM LES



Modelling number concentrations over Paris

- Estimate number emissions from local emission inventory for July 2009 + UFP/PM emission ratio from UK Bottom-Up inventory (Sartelet et al. ACP 2022)
- Spatial resolution of 2 km x 2 km
- The nucleation parameterization of organics from monoterpenes autoxidation/sulfuric acid/water (heteromolecular) performs better than ammonia/sulfuric acid/water (ternary) or sulfuric acid/water (binary)
- *Further work for more recent years and using Street-in-Grid modeling (CHIMERE/SSH-aerosol/MUNICH) – Link to WP4.3*



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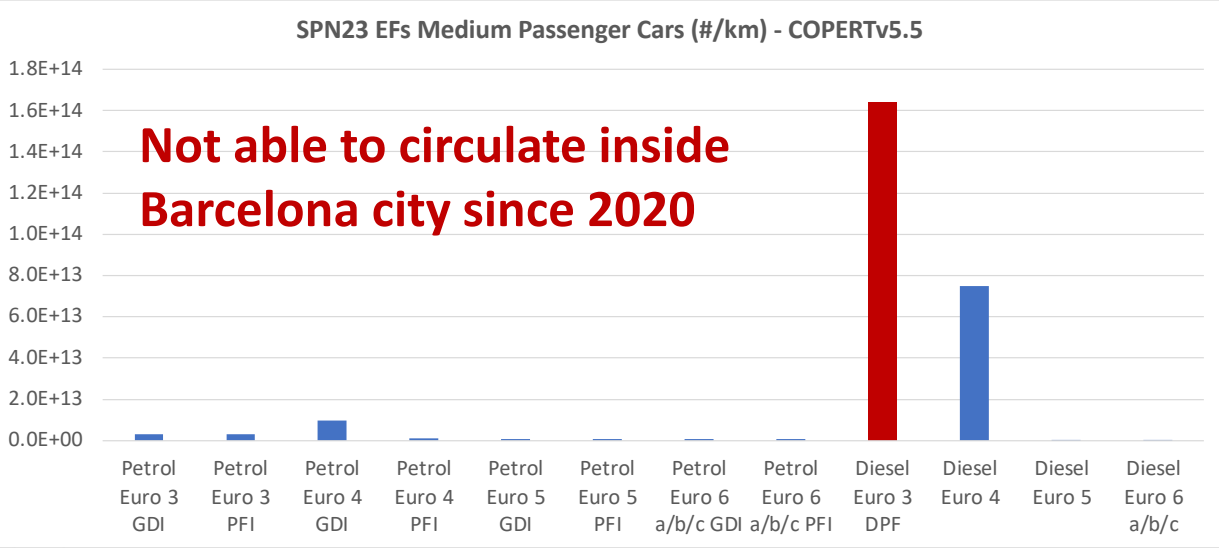
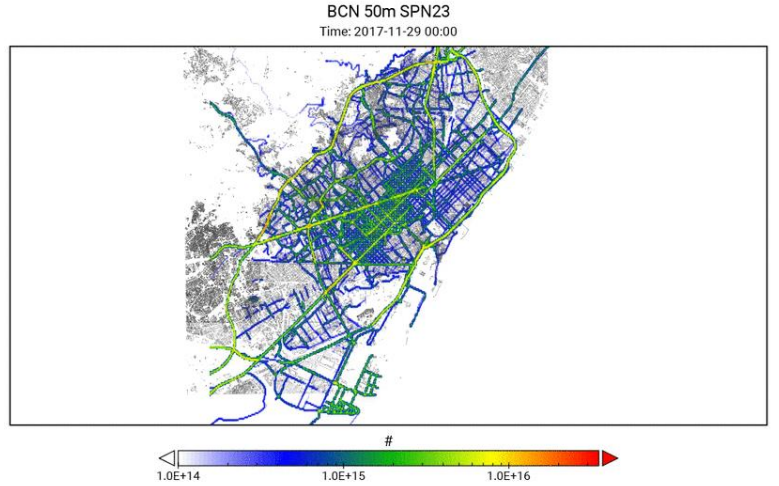
Constraining BC/UFP emissions at the road-link level for Barcelona

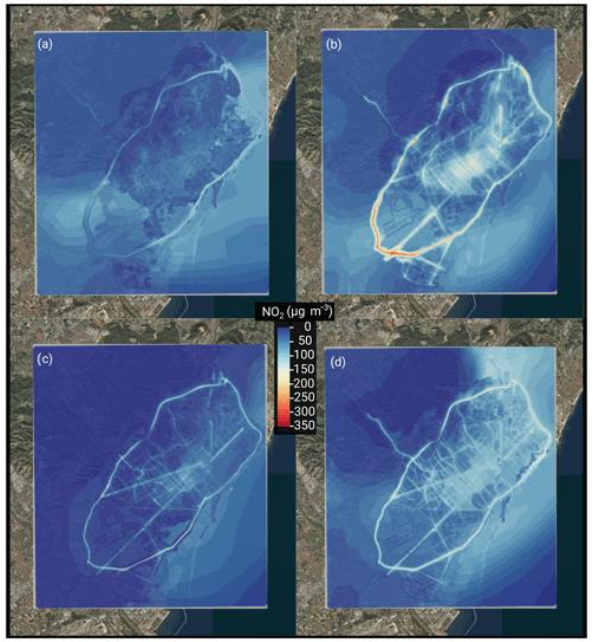
- Inclusion of UFP road transport emissions in HERMESv3 (Guevara et al., 2020) using the new COPERTv5.5 exhaust EFs as reported by EMEP/EEA guidelines (SPN23 EFs per vehicle category).
  - ***Large differences between Euro categories (impact of Low Emission Zone?)***
  - *The lower cut-off set by the Euro standards (23nm) means that more than ~30% of the smallest UFP in urban environments may not be included (Wehner and Wiedensohler, 2003)*





Constraining BC/UFP emissions at the road-link level for Barcelona

- Use of the CALIOPE-Urban modelling system (Benavides et al., 2019) combined with BC campaign (horizontal and vertical profiles) (Amato et al., 2019) and UFP measurements derived from WP4



Benavides et al. (2019)

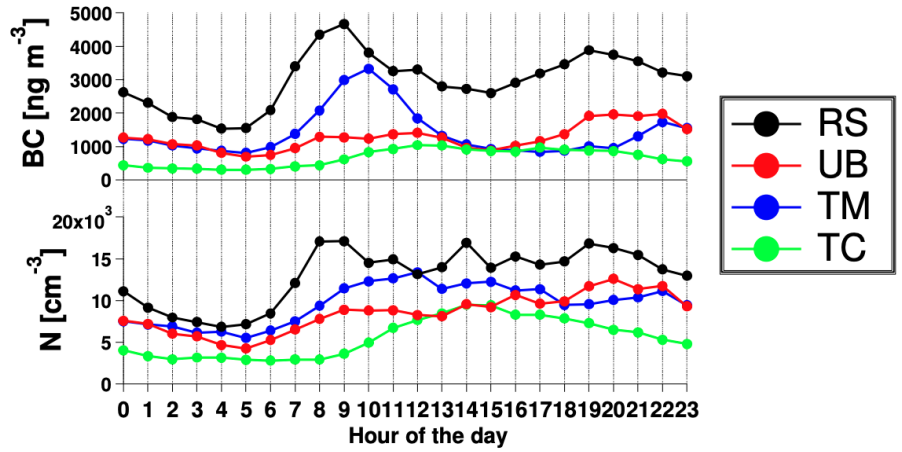
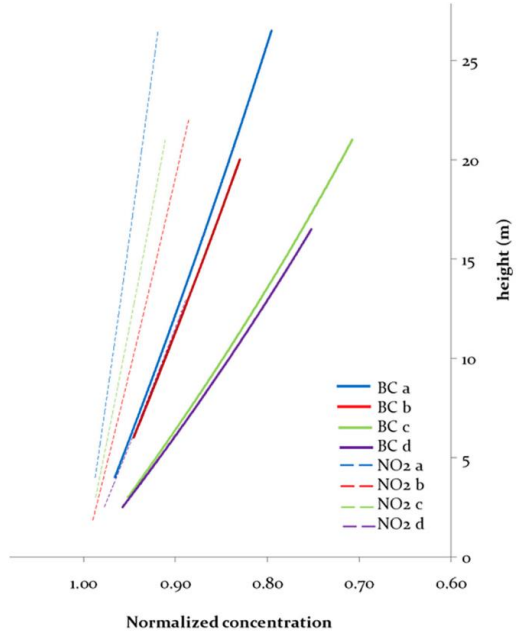


Fig. 1. Diurnal profile of BC and *N* at four different monitoring sites.

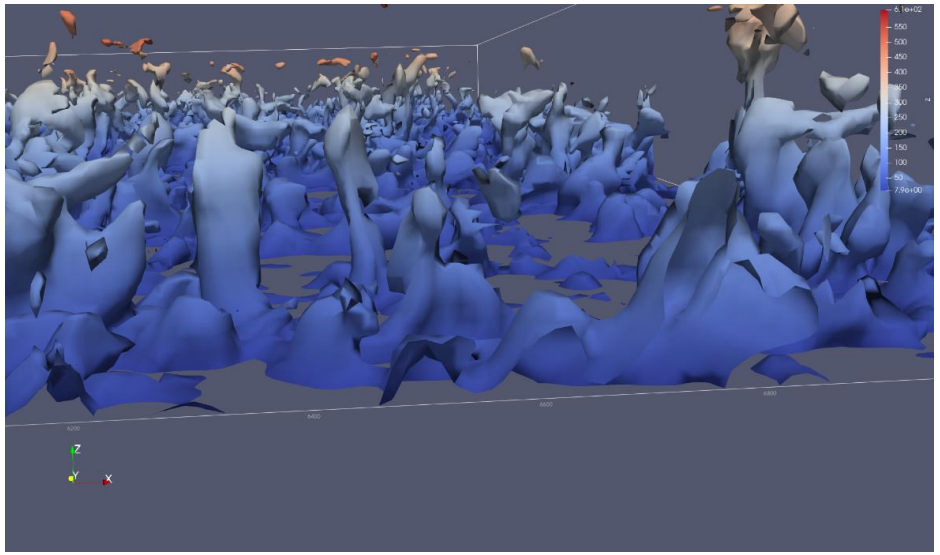
Dall'Osto et al. (2013)



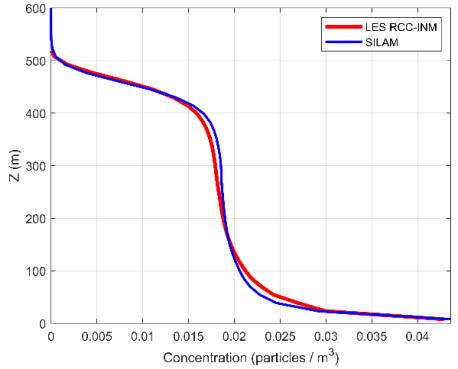
Amato et al. (2019)

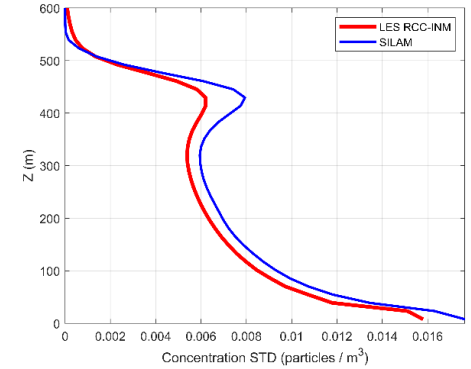
LES-SILAM passive tracer test

- Technical sanity check
  - Example: Isosurface of concentration
  - 60-sec self-decaying tracer
  - convective boundary layer
  - color shows height, [m].
  - Horizontal resolution 15 m



- Quantitative evaluation
  - Passive 920-sec self-decaying tracer
  - mean vertical profile (left)
  - standard deviation of vertical profile (right)





  - SILAM was run without diffusion → higher variability
  - LES transport scheme is diffusive

PALM LES to SILAM interface

Technical sanity check

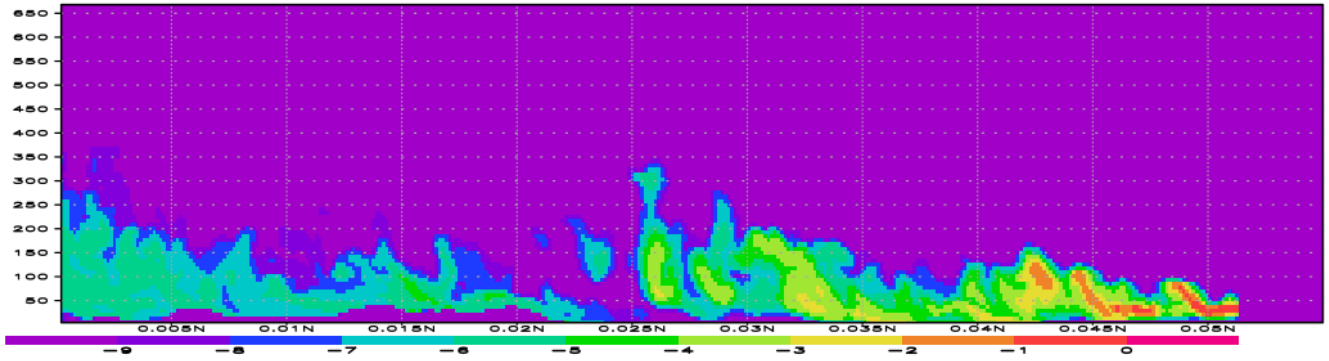
- Passive-tracer plume from elevated source
- 16-m resolution over orography
- City of Turku
- Neutral boundary layer

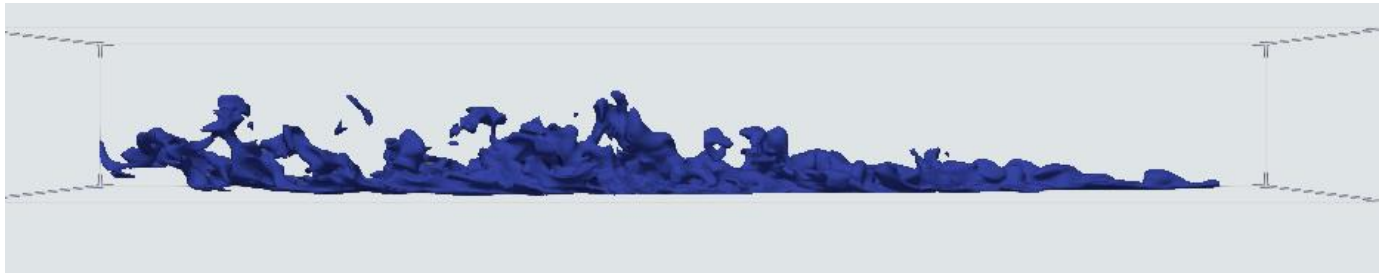
Qualitative evaluation

- Realistically-looking plume
- No artifacts due to “missing cells”

Further steps:

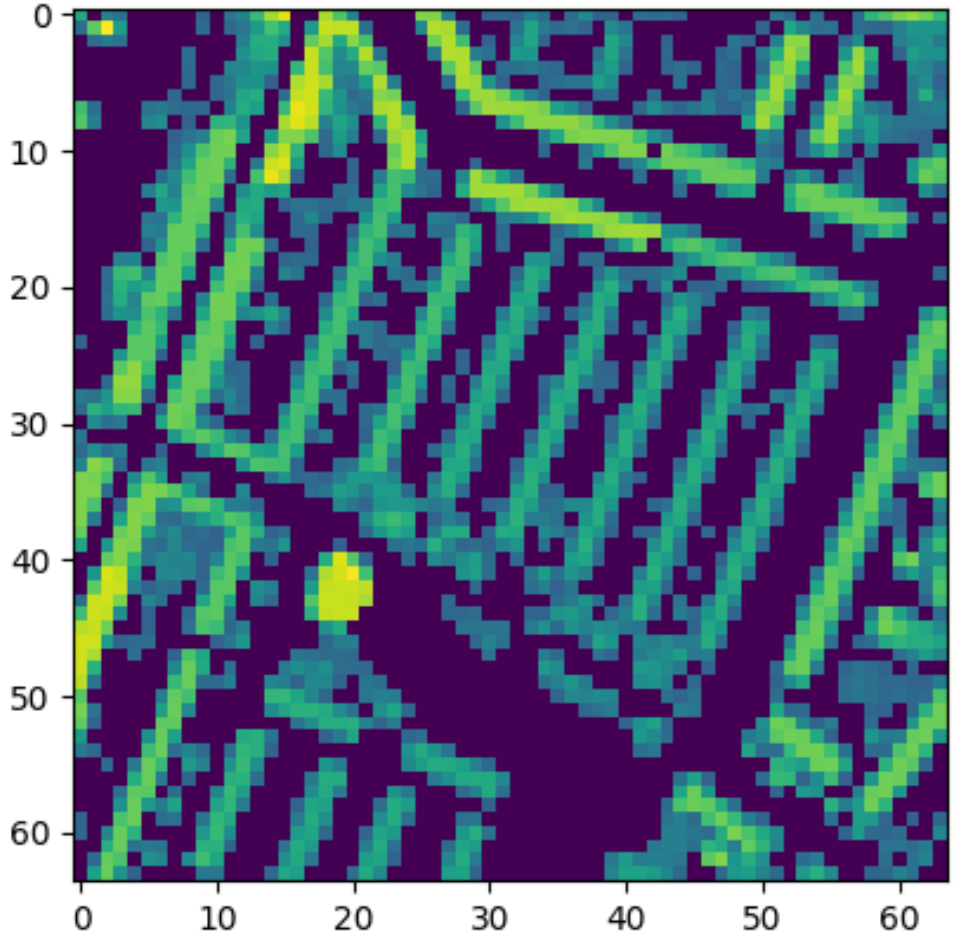
- 3D emissions
- Full chemistry





Case Rotterdam, NL

- DALES implementation of Rotterdam urban canopy, Stephan de Roode, Pam Witsenboer (TU-Delft)



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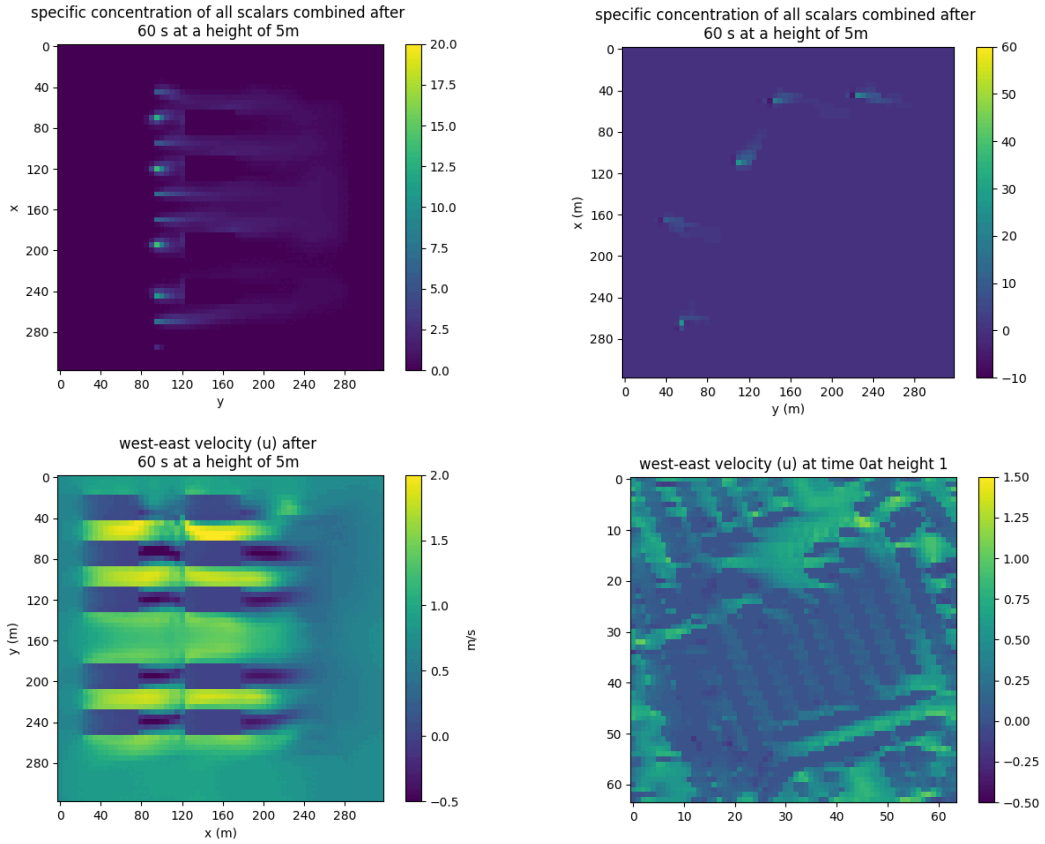

Information about the run

- Runtime: 10800 s
- 5 scalars
- Domain: 320 m x 320 m
- Grid points: 64 x 64
- $\Delta x = \Delta y = 5$ m
- Advection scheme kappa used for scalar concentration
- Strip function used

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Concluding Remarks and Way forward

- High resolution modelling tools being developed to improve characterization of urban dispersion
- Next steps will include evaluation of these models against measurements to improve urban aerosol particle emissions
- Emission datasets developed in T3.2 will be considered as input