Local-scale air quality modeling in the urban street canyon

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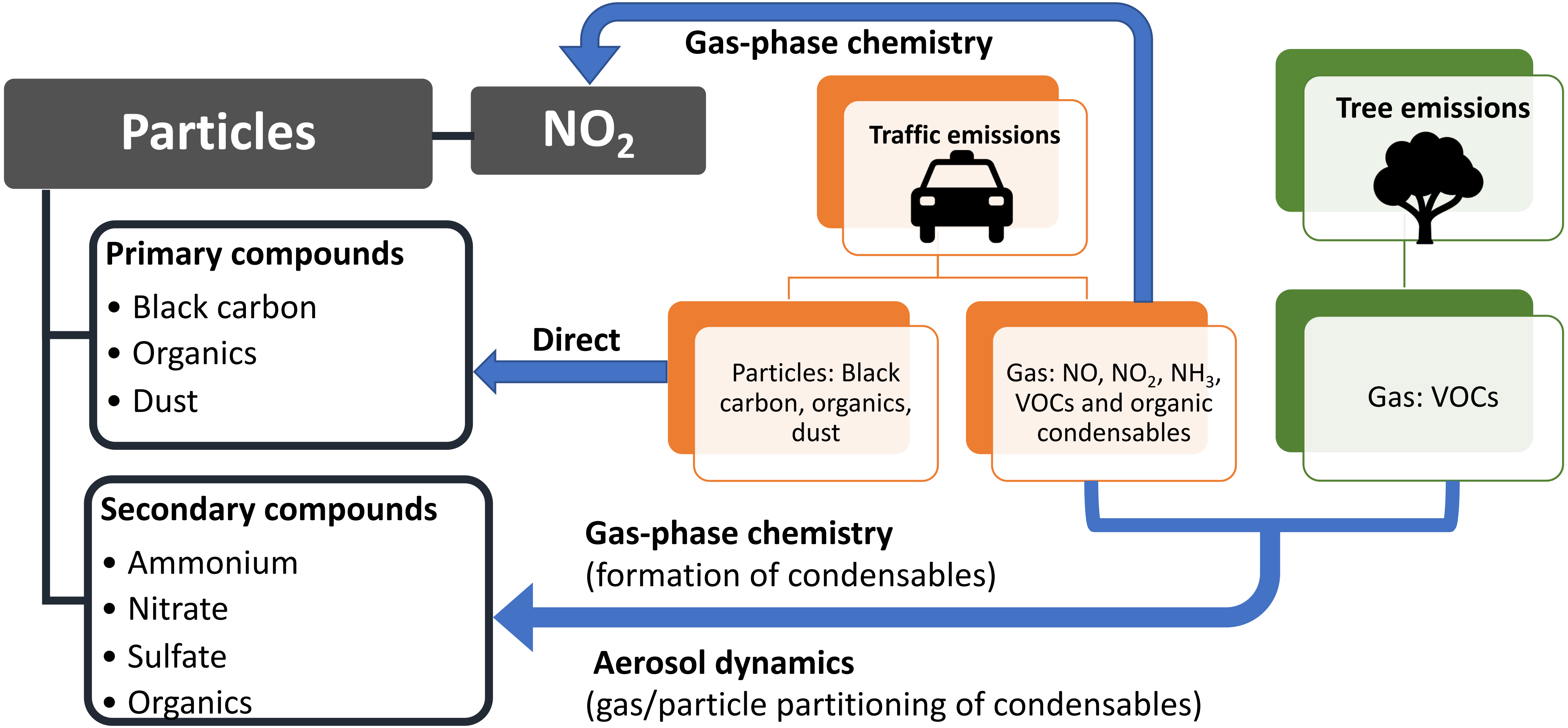
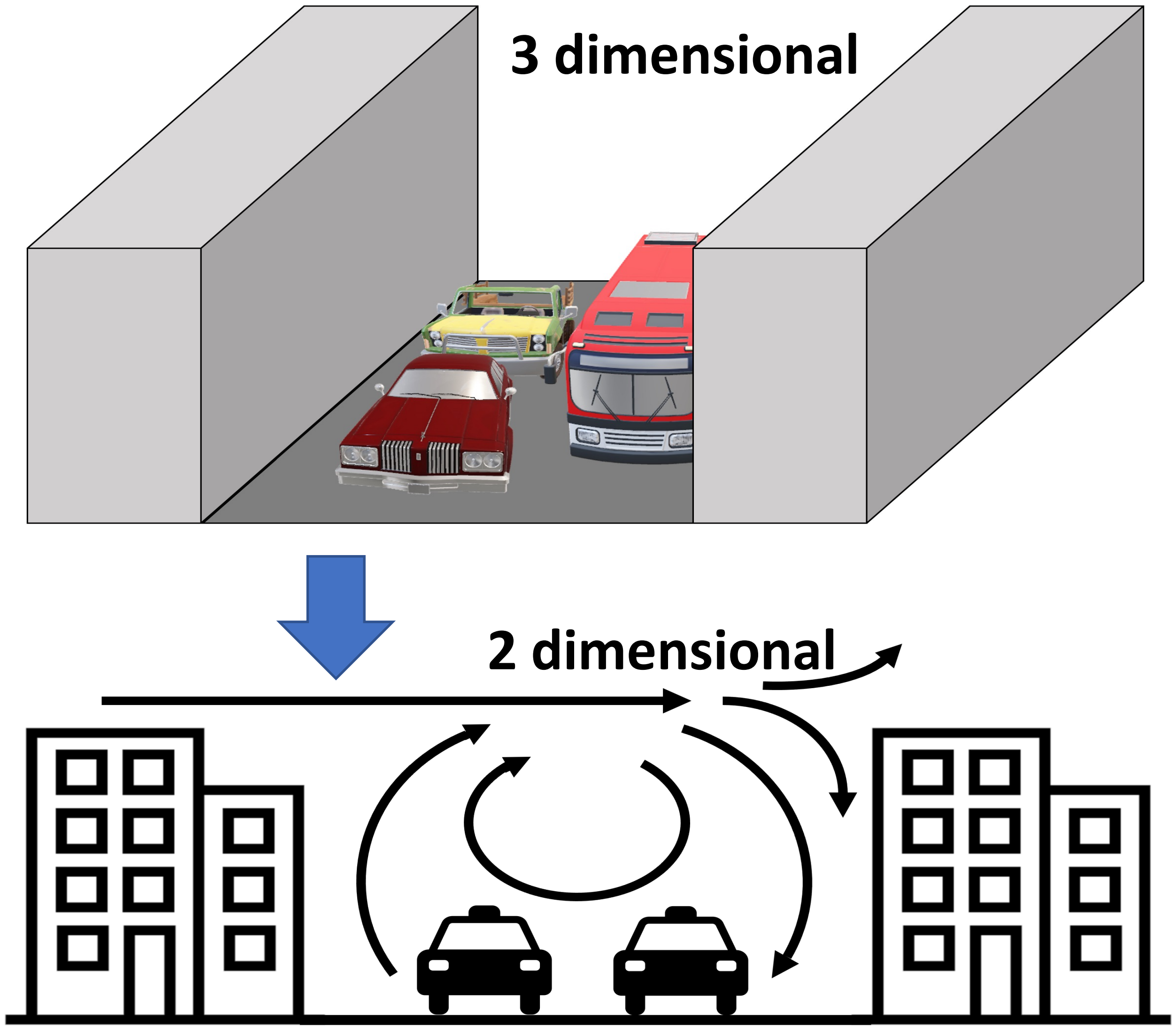
Introduction – Street emissions and concentrations



Objectives: Reproduce concentrations of gaseous and particle pollutants and study the impact of chemistry on their fomation

Model presentation



Use simplified street canyon as workbench to investigate the impact of chemistry on the air quality

- 2D modelling of street canyon
- Simulation of atmospheric dispersion, gas chemistry and aerosol dynamics
- Comparison of different CFD tools coupled to chemistry model (collaboration with Tokyo University)

Model presentation

CFD model:

Code_Saturne

code_saturne

OpenFoam

OpenFOAM

RANS model   k-ε linear production (CS)

RNG k-ε model (OF)

Coupling

Chemistry model:

SSH-aerosol – gas-phase chemistry and aerosol dynamics

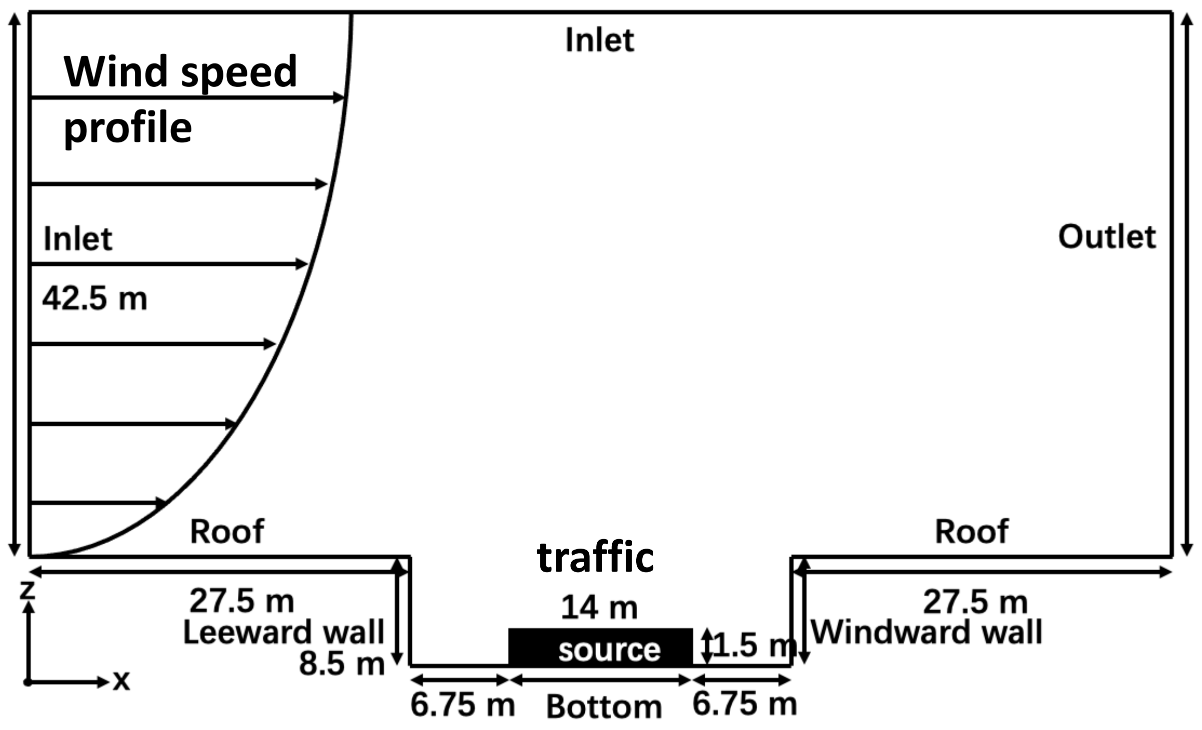
SSH aerosol

- Gas-phase chemistry: **Modified CB05** (Carbon Bond mechanism version 5)
- Aerosol dynamics: Condensation/evaporation, coagulation

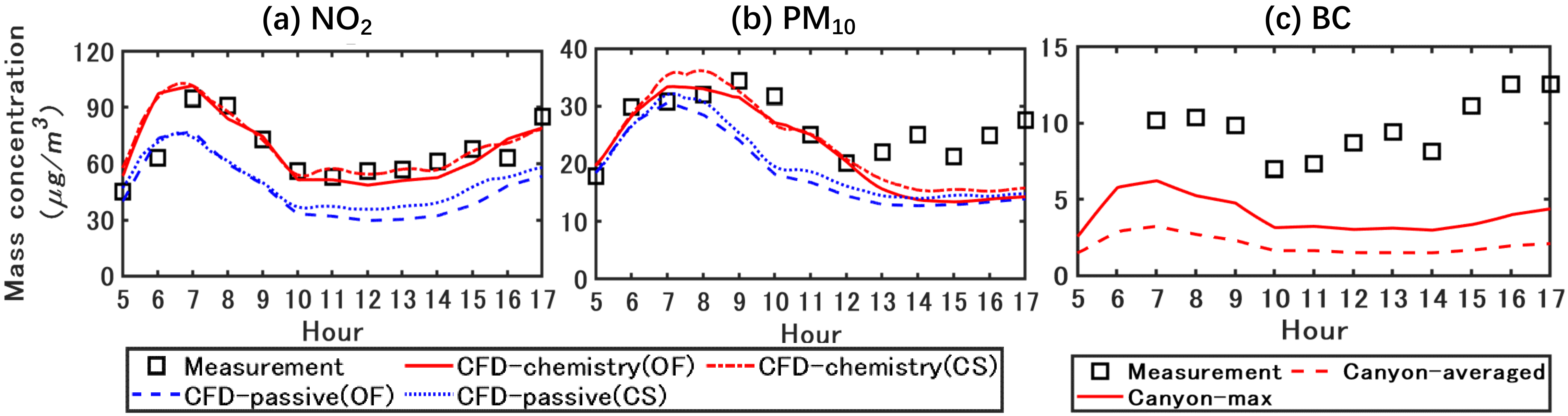
Model setup

Field measurements & simulation set-up

- Measurement of **NO_2, PM_{10}** and **Black Carbon (BC)** concentrations at a street station (ANR Traffipollu).
- Period: April 30 04:30-17:00 (Local time)
  Measured wind direction perpendicular to the street
- Location: Boulevard Alsace-Lorraine (Le Perreux sur Marne, Greater Paris)
- Traffic emissions (Kim et al 2022, GMDD)
- Background concentration (Sartelet et al. 2018, Atmos. Environ.)
- Meteorological boundary conditions (Lugon et al 2021 GMD)

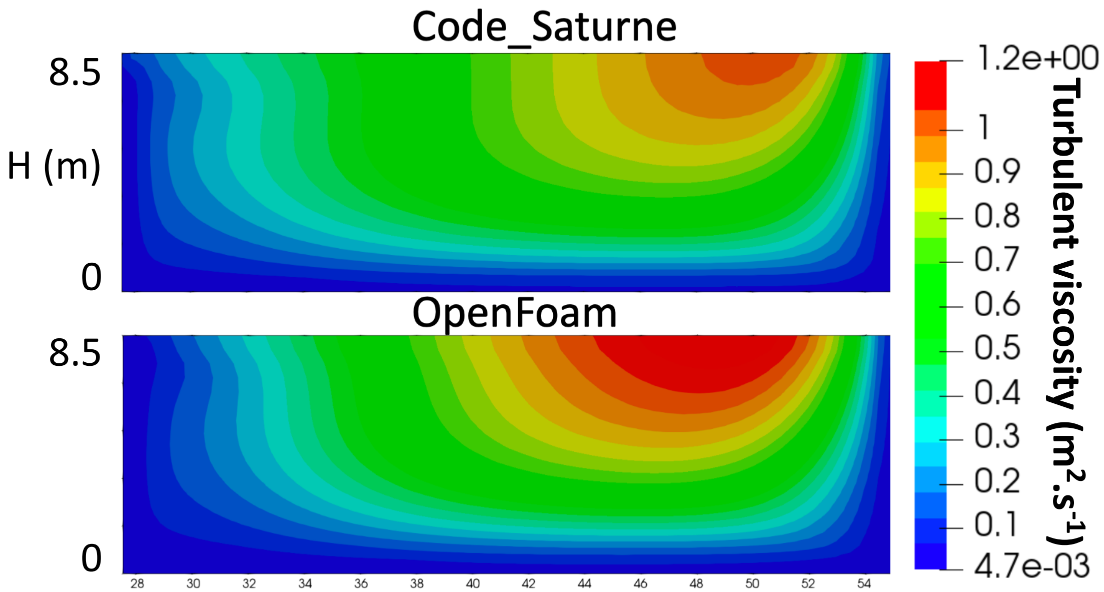


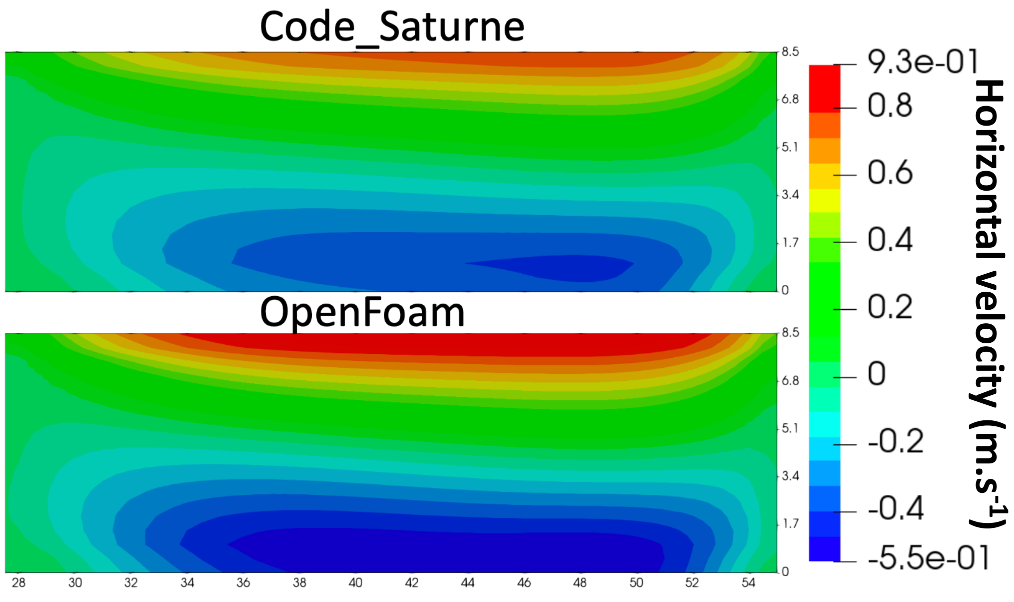
Model validation

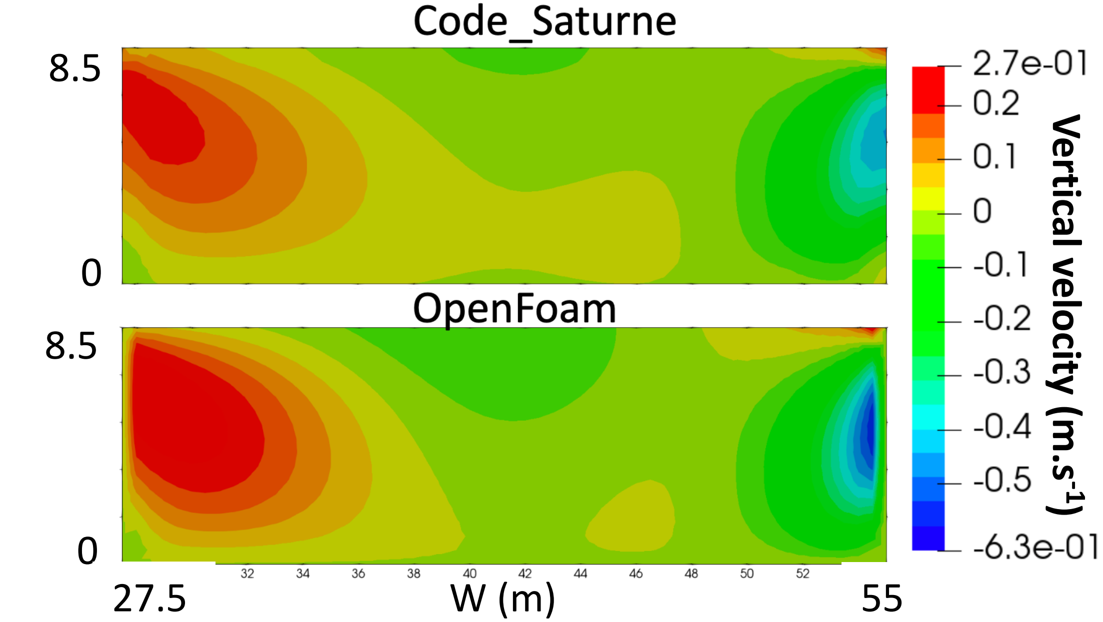


- For NO_2: good agreement with observations in the daytime
- For PM_{10}: good agreement with observations in the morning, but under-estimation of the concentrations in the afternoon because of under-estimation of background concentrations (Lin et al. ACP 2022)
- For black carbon: under-estimation because of under-estimation of non-exhaust tire emission factors (Lugon et al. GMD 2021)

Comparison of flow field in two CFD models





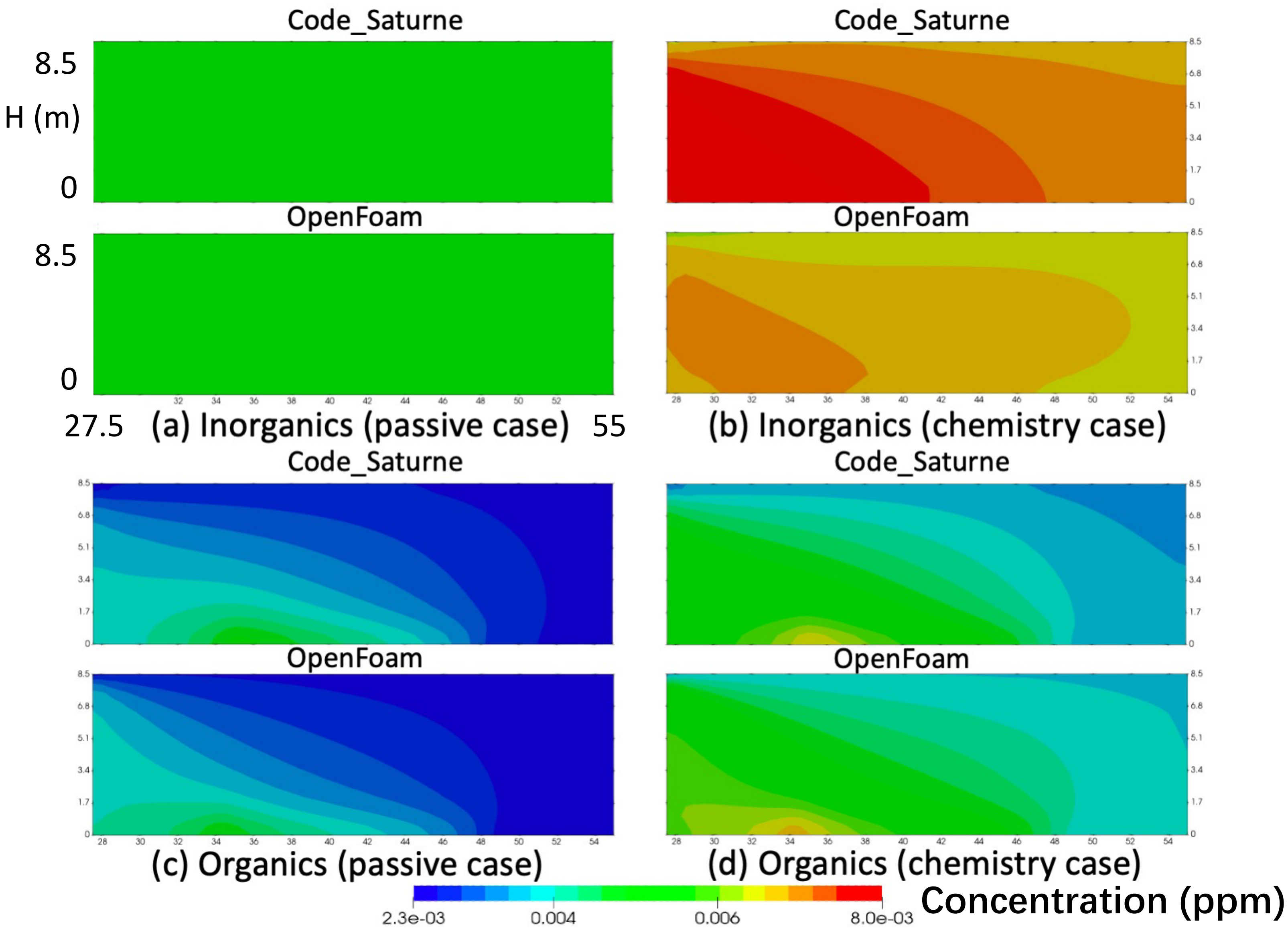


Different choice of turbulent models in two CFD tools:

- Slight difference in turbulence and velocity fields

⇒ Difference in species dispersion

Comparison of concentration field in two CFD models



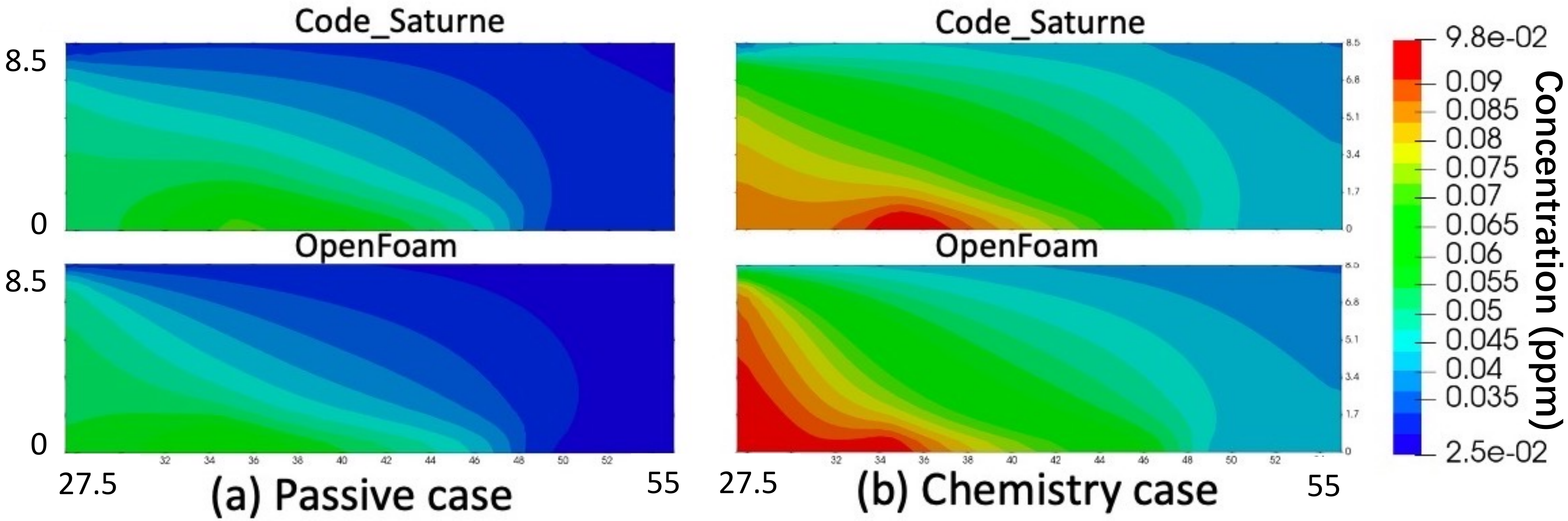
-Background consistency in two CFD models

-Different turbulent models impact the dispersion of emitted pollutants

-Slight difference in inorganic and organic aerosols concentrations

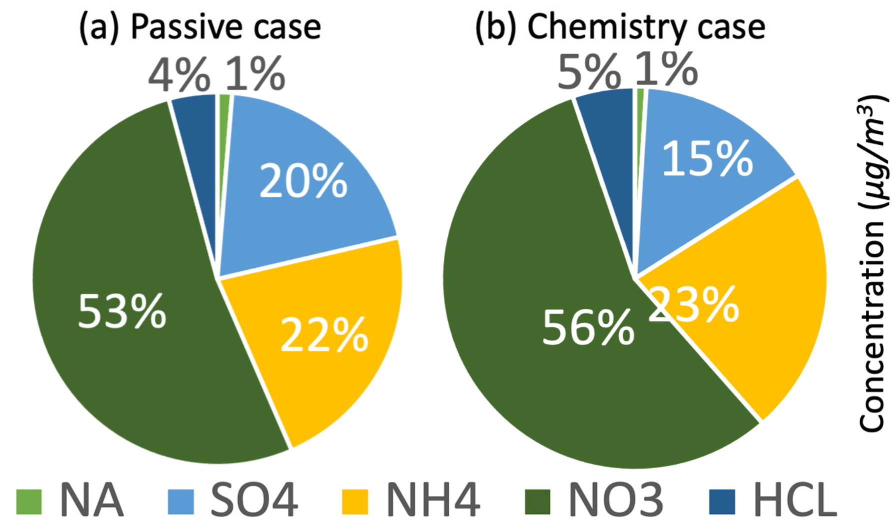
-Chemistry impact significantly the formation of inorganic and organic aerosols

Impact of chemistry for NO_2

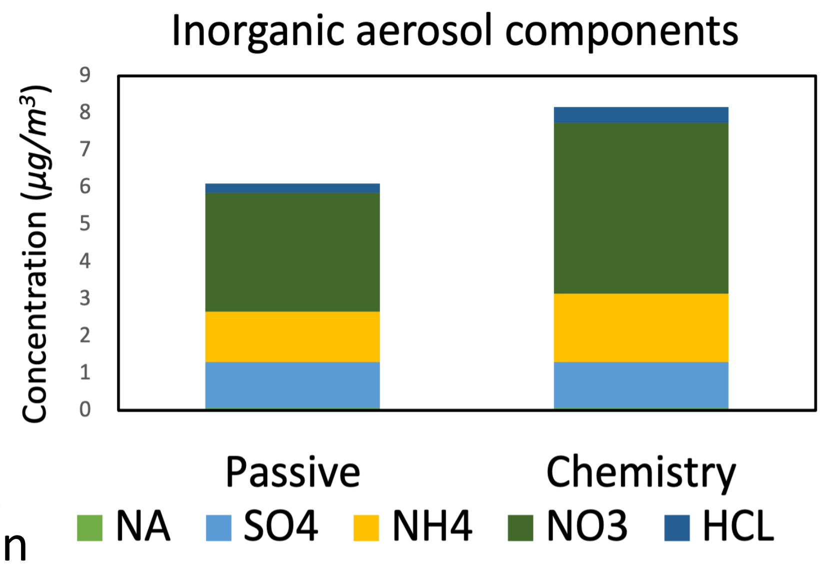


- Gas chemistry leads to an average increase of NO_2 by 40.5% in Code_Saturne and 46.7% in OpenFoam
- Larger concentrations are found in the street near the leeward wall due to the reverse flow
- NO_2 mainly increased due to gas-chemistry production from NO (emission)and O_3 (background).

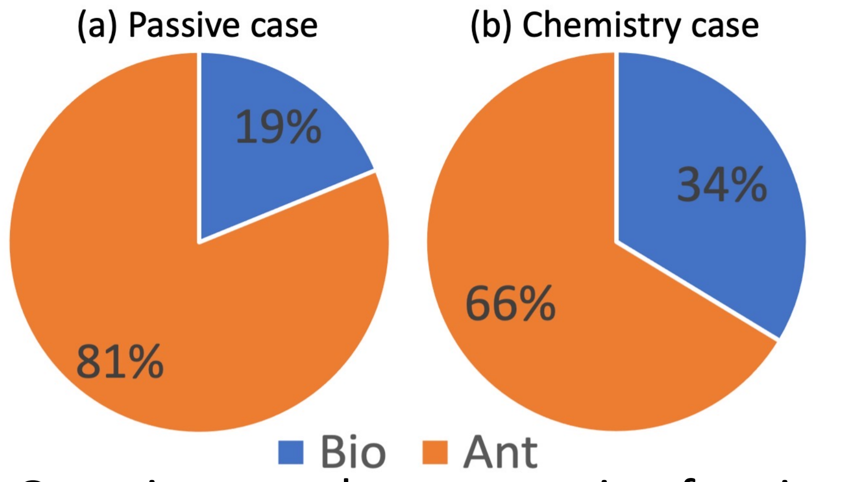
Impact of chemistry for inorganic and organic aerosols



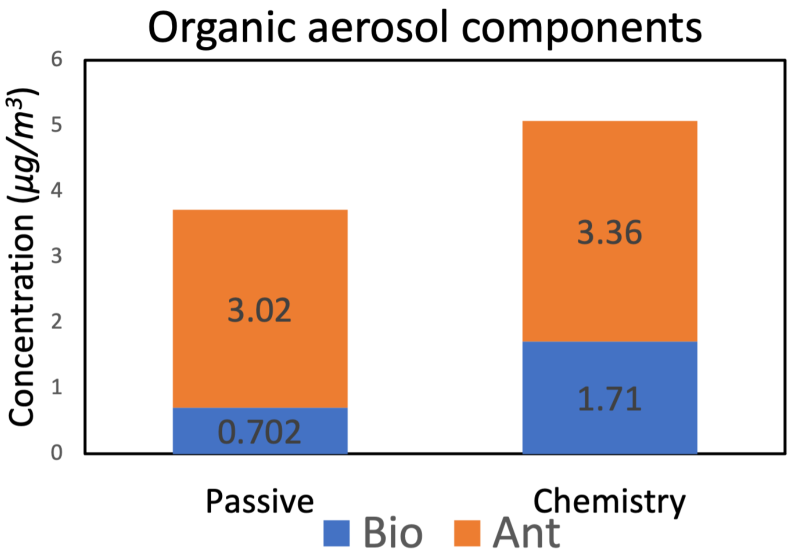
Inorganic aerosol concentration fraction



- Increase of inorganic aerosols mainly comes from ammonium nitrate (NH_4, NO_3)
- NH_4, NO_3 increase because of the emission of NH_3 gas and aerosol dynamics



Organic aerosol concentration fraction



- Increase of organic aerosols mainly comes from biogenic organic aerosols (formed from mono-terpene, isoprene, etc)
- Increase of ammonium nitrate enhances the condensation of hydrophilic species (biogenic)

Conclusions

- A local-scale air quality model is developed by coupling CFD (Code_Saturne, OpenFoam) to chemistry model (SSH-Aerosol)
- The model is validated by comparing with measurements
- Similar results obtained from Code_Saturne/SSH-Aerosol and OpenFoam/SSH-aerosol simulations
- Gas chemistry and aerosol dynamics influence NO_2 and inorganic and organic aerosol concentrations

References

[1] Kim, Y. et al., MUNICH v2.0: a street-network model coupled with SSH-aerosol (v1.2) for multi-pollutant modelling. Geosci. Model Dev. in review.
[2] Lugon, L. et al., Black carbon modeling in urban areas: investigating the influence of resuspension and non-exhaust emissions in streets using the Street-in-Grid model for inert particles (SinG-inert), Geosci. Model Dev.
[3] Sartelet, K et al., 2018. Emission of intermediate, semi and low volatile organic compounds from traffic and their impact on secondary organic aerosol concentrations over Greater Paris. Atmos. Environ.
[4] Lin, C. et al., Modelling of street-scale pollutant dispersion by coupled simulation of chemical reaction, aerosol dynamics, and CFD. Atmos. Chem. Phys. Discuss. in review.

Thank you for your attention