

## Development and Application of an Online Coupled Chemistry Model Embedded in the Urban Microscale Model PALM-4U - First results for Berlin, Germany

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**Abstract:** Accurate representation of emission, dispersion, chemical transformation and removal of air pollutants in the urban canopy requires fine-scale turbulence-resolving simulations that can explicitly resolve building structures, surface heat fluxes at building facades, street canyons and terrain variations. Large Eddy Simulation (LES) models permit to resolve relevant scales of turbulent motion, so that these models can capture the inherent unsteadiness of atmospheric turbulence. However, LES models are so far barely applied for urban air quality studies, in particular chemical transformation of pollutants. A new highly efficient state-of-the-art urban microscale model, PALM-4U, has been developed that includes both gas-phase and aerosol chemistry. The LES model PALM (Maronga et al., 2015) serves as the core for PALM-4U. A fully coupled 'online' chemistry model has been implemented into PALM-4U for gas-phase chemistry while the sectional aerosol model SALSA (Kokkola et al., 2008) is also available for aerosol chemistry. The latest version of the Kinetic PreProcessor (KPP), Version 2.2.3, has been utilized for the numerical integration of gas-phase chemical reactions. Due to the high computational demands of LES and chemistry models, a reduced chemistry mechanism was implemented which includes only major pollutants namely O<sub>3</sub>, NO, NO<sub>2</sub>, CO, a highly simplified VOC chemistry and a small number of products. A full complex chemistry is available together with the computationally less-demanding Reynolds-Averaged-Navier-Stokes (RANS) mode of PALM-4U. In this work, we present model results for an area in central Berlin at an ultra-high resolution of 1.0 meter. The model considered emissions from street canyons and selected point sources. Results show transport, gas-phase reactions and removal of atmospheric pollutants. The model has also been evaluated against observed concentrations of chemical species.

### References:

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