Evaluation of chemical mechanisms implemented in the microscale urban climate model PALM-4U

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Large Eddy Simulation (LES) models have proven to be effective tools to simulate urban canopy features more accurately compared to Reynolds Averaged Navier-Stokes (RANS) models. Currently, most of the atmospheric pollutant dispersion and air quality models are based on parameterizations. However, at the urban scale these models are unable to accurately resolve turbulence, building structures and pollutant dispersion. In this work we have employed a state-of-the-art microscale urban climate model - PALM-4U, that is feasible to simulate a variety of urban features such as the urban heat island, ventilation in street canyons, and pollution hotspots etc. PALM-4U is based on the well-established LES model PALM (Maronga et al., 2015). A fully coupled 'online' chemistry model has been implemented into PALM-4U which includes both gas-phase and aerosol chemistry. The model utilizes Kinetic PreProcessor KPP, Version 2.2.3 (Damian et al., 2002), to generate code for the numerical integration of the gas phase chemistry. Aerosol processes are described by the sectional aerosol model SALSA (Kokkola et al., 2008), (https://palm.muk.uni-hannover.de/trac/wiki/doc/app/salsa). A dominant feature of the chemistry module is its flexibility in the choice of the chemistry mechanism. The user can virtually implement any mechanism (subject to availability of the desired computational power) for transport and chemical transformation of species. However, PALM-4U, also provides several gas-phase chemistry mechanisms of different complexity. Four different chemical mechanisms, namely, SIMPLE, CBM4, SMOG (a reduced chemistry mechanism, which includes only O_3, NO, NO_2, a highly simplified VOC chemistry and a small number of products) and PHSTAT (photo-stationary equilibrium) have been evaluated against observed trace gases and aerosol data of various air pollutants in the urban canopy. The model simulations are run over an area in the central Berlin, Germany at a resolution of 10 meters. PALM-4U is forced by meteorological boundary conditions from a regional scale model COSMO (Consortium for Small-scale Modelling). The model considers emissions from street canyons and selected point sources. The model performance evaluation results for the four chemical mechanisms are presented.