



## **Test of gas phase chemistry mechanisms for a LES model with online coupled chemistry**

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To accurately simulate dispersion, chemical transformation and removal of air pollutants in the urban canopy layer, fine-scale turbulence-resolving simulations are required that can explicitly resolve building structures and street canyons. Large-Eddy Simulation (LES) models explicitly resolve the dominant scales of turbulence in the atmospheric boundary layer and therefore, have the potential to capture the turbulent motion within street canyons as well as the observed short term fluctuations of pollutant concentrations. LES models including chemical transformation of pollutants are so far barely applied for urban air quality studies. Within the joint project MOSAIK (Model-based city planning and application in climate change) a new urban microscale model including gas phase chemistry and aerosols, PALM-4U, has been developed. The state-of-the-art LES model PALM (Maronga et al, 2015, Geosci. Model Dev., 8, doi:10.5194/gmd-8-2515-2015) is used as core model for PALM-4U. In order to obtain the necessary flexibility in the choice of the chemistry mechanisms the gas-phase chemistry was implemented using the Kinetic PreProcessor KPP. Due to the very high computational demands of an LES-based model, compromises are required with respect to the degree of detail of the gas-phase chemistry mechanisms. A number of chemical mechanisms with varying complexity and detail that ranges from a strongly reduced mechanism which includes only a simple  $O_3$ - $NO_2$ - $NO$ - $VOC$ - $HO_x$  chemistry and a small number of products to large mechanisms which are typically used in regional air quality models were implemented into PALM-4U. The performance of different gas-phase chemistry schemes of different complexity within the LES model PALM-4U is tested and compared.