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Development and Implementation of an Online Chemistry Module to a Large Eddy Simulation Model

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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 and advection. However, LES models are so far hardly applied for urban air quality studies, in particular chemical transformation of pollutants. Within the BMBF (Bundesministerium für Bildung und Forschung) funded joint project MOSAIK (Modellbasierte Stadtplanung und Anwendung im Klimawandel / Model-based city planning and application in climate change) the state of the art LES model PALM (Parallelized LES Model; Maronga et al, 2015, Geosci. Model Dev., 8, doi:10.5194/gmd-8-2515-2015) is extended by an atmospheric chemistry scheme. Due to the high computational demands of a LES based model, compromises in the description of chemical processes are required. Therefore, a reduced chemistry mechanism, which includes only major pollutants namely O_3, NO, NO_2, CO, a highly simplified VOC chemistry and a small number of products have been implemented. For practical applications, our approach is to go beyond the simulation of single street canyons to chemical transformation, advection and deposition of air pollutants in the larger urban canopy. Tests of chemistry schemes and initial studies of chemistry-turbulence interactions are presented.