

Development and Implementation of an Online Chemistry Module to a Large Eddy Simulation Model for the Application in the Urban Canopy

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Adequate modelling tools are required to support urban planning and the development of strategies aiming at minimizing climate change-related vulnerabilities and risks of human inhabitants such as poor air quality. However, a realistic implementation of urban canopy processes still poses a serious challenge for current air quality models owing to the small scale of the phenomena to be described.

Large-Eddy Simulation (LES) models explicitly 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 when the chemical transformation of pollutants is involved.

Within the BMBF funded joint project MOSAIK (Model-based city planning and application in climate change) the state of the art LES model PALM is extended by an atmospheric chemistry scheme. Due to the high computational demands of an LES based model, compromises in the description of chemical and removal processes are required. A computationally less-demanding RANS mode of the model will also be developed. Chemistry modules of different complexity for both the LES and the RANS mode have to be supplied for practical applications. Therefore, gas-phase chemistry has been implemented using the Kinetic PreProcessor (KPP) in order to obtain the necessary flexibility in the choice of the chemistry mechanism.

For the LES mode 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 is implemented while for the RANS mode a full complex chemistry module is available.

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.