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Test of gas phase chemistry mechanisms and boundary conditions for the LES model PALM-4U with online coupled chemistry

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Introduction

Increasing urbanization has a negative impact on local climate and air quality due to urban soil sealing and consumption of resources like fossil fuel. Adequate modelling tools are required to support urban planning and the development of strategies aiming at minimizing adverse effects on urban climate and air quality. Although Large-Eddy Simulation (LES) models can capture the transient flow structures of atmospheric turbulence and advection by explicitly resolving relevant scales of turbulent motion, these models are rarely used for urban climate and air quality studies.

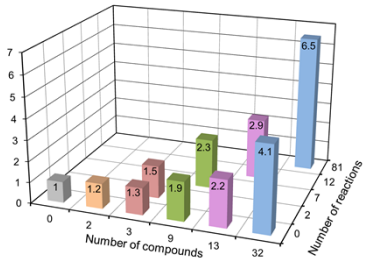
Within the joint project MOSAIK (Modellbasierte Stadtplanung und Anwendung im Klimawandel/Model-based city planning and application in climate change), the micro-scale urban climate model PALM-4U has been developed under the lead of the Institute of Meteorology and Climatology at the Leibniz Universität Hannover (Maronga et al., 2019). PALM-4U, which is based on the Parallelized Large-Eddy Simulation Model PALM (Maronga et al, 2015) includes among others online coupled gas phase chemistry and the sectional aerosol module SALSA (Kurppa et al., 2019).

Chemistry implementation into PALM-4U

- Automatic generation of the chemistry code with the Kinetic Pre-Processor (KPP) allows for high flexibility in the choice of gas phase chemical mechanisms. A vectorized version is also available.
- Automatic adaptation of KPP generated code for PALM-4U based on the KP4 preprocessor (Jöckel et al., 2010).
- Choice of pre-processed mechanisms of different complexity: Passive tracers, photo-stationary equilibrium (PHSTAT), simple photochemistry mechanisms with 7 and 12 reactions (SIMPLE, SMOG), CBM4. Option for adding user-specified mechanisms.
- Photolysis frequencies are currently parameterized following the MCM (Master Chemical Mechanism, Saunders et al., 2003).
- Gas phase chemistry coupled with the aerosol model SALSA (Kurppa et al, 2019).
- Dry deposition.
- Anthropogenic emissions options:
  - Gridded NetCDF files (two levels of detail)
  - Parameterized traffic emissions depending on street type from OpenStreetmap and typical emission factors from HBEFA 3.3.
- Lateral boundary conditions for chemistry:
  - Cyclic (typical for LES)
  - Fixed boundary conditions
  - Time dependent boundary conditions from WRF-Chem.

Performance of the chemistry module

Due to the high computational demands of LES, compromises are necessary with respect to the degree of detail of the atmospheric chemistry. Test simulations with 10 m grid width for a 1 km x 1 km area in Berlin have shown that the computation of the transport of the chemistry compounds is more time consuming than the computation of the chemical reactions.



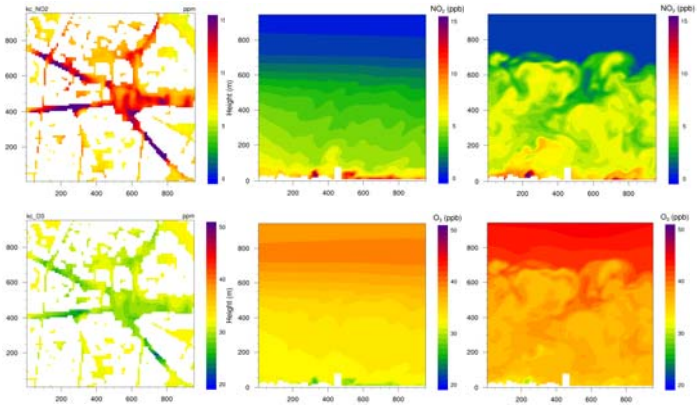
CPU time requirement of the mechanisms implemented in PALM-4U: PASSIVE (orange), PHSTAT (red), SIMPLE (green), SMOG (purple) and CBM4 (blue) relative to a meteorology only run (gray). The bars in the front show the increase time if only the transport of the chemical compounds is considered.

Nesting with boundary conditions from WRF-Chem

Cyclic boundary conditions are frequently applied in LES in order to obtain lateral boundary conditions for the turbulent quantities. To account for variable weather conditions and regional scale pollutant transport PALM-4U allows time-dependent boundary conditions from regional models. Turbulent fluctuations, which are not provided by the regional simulation but are needed as additional boundary conditions for the LES model are produced by a turbulence generator.

Due to the lateral forcing the boundary layer top is less pronounced in the nested case than for cyclic boundary conditions.

Nested, BCs from WRF-Chem **Cyclic BCs**



Simulation with boundary conditions from WRF-Chem for a 1 km² area of Berlin around the Ernst-Reuter-Platz, a junction with some high buildings and heavy car traffic (95 x 95 grid points and 10 m grid width): Simulated concentrations of NO_2 (top) and ozone (bottom) on July 29 2017, 10 h.

Same as left, but with cyclic boundary conditions. Cyclic BCs can lead to unrealistic accumulation of pollutants in areas strong sources.

Concluding remarks and outlook

PALM-4U is able to simulate resolved turbulence and chemical transformations – also allowing for more comprehensive chemical mechanisms then shown here – in the urban environment. It permits also to simulate chemical transformation, advection and deposition of air pollutants in the larger urban canopy. The use of lateral boundary values of mean quantities from mesoscale models such as COSMO or WRF-Chem allows to consider the effect of regional pollutant transport.

PALM-4U is still under further development, which also holds for its chemistry module. Work is in progress to add new features such as more comprehensive photolysis schemes and inclusion of shading effects on photolysis, biogenic VOC emissions, and wet deposition.

References

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