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Test of chemistry boundary conditions for large-eddy simulations of urban areas

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Introduction

Large-Eddy Simulation (LES) allow to simulate pollutant dispersion at a fine-scale with explicitly resolved turbulent transport around building structures and in street canyons.

Within the collaborative project MOSAIK (Model-based city planning and application in climate change) the LES based microscale urban climate model with atmospheric chemistry PALM-4U (i.e. PALM for Urban applications) has been developed (Maronga et al., 2019, Maronga et al., 2020).

Usually, cyclic boundary conditions are applied in LES in order to obtain lateral boundary conditions for the turbulent quantities. In order to allow also for variable weather conditions PALM-4U includes a preprocessor which supplies boundary conditions from COSMO output. To account for regional scale pollutant transport chemistry boundary conditions from a regional simulation with WRF-Chem were added.

Chemistry in PALM-4U

- **Chemistry implementation:**
  - Flexible automatic generation of gas phase chemistry code with the Kinetic Pre-Processor (KPP) and adaptation of the KPP generated code for PALM-4U based on the KP4 preprocessor (Jöckel et al., 2010). A vectorized version is also available.
  - Choice of pre-processed mechanisms of different complexity: Passive tracers, photo-stationary equilibrium, two simple photo-chemistry mechanisms with 7 and 12 reactions, and CBM4. Option for adding user-specified mechanisms.
  - Gas phase chemistry coupled with the aerosol model SALSA (Kurppa et al, 2019).
  - Photolysis frequencies (currently parameterized following Saunders et al., 2003) and 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 (frequently applied for LES)
  - Fixed boundaries from initial conditions
  - Time dependent boundary conditions e.g. from WRF-Chem.

Simulation setup

PALM-4U simulations with cyclic boundary conditions and with time dependent boundary values for the meteorological variables, NO, NO_2 and ozone from WRF-Chem ('offline nested run') were performed for a small part of Berlin around the Ernst-Reuter-Platz, an area with some high buildings and heavy car traffic. The tests were made for a 2 x 2 km^2 domain with 200 x 200 x 320 grid points and 10 m grid width and photostationary equilibrium chemistry.

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 (Maronga et al., 2020).

References

MOSAIK web page: https://palm.muk.uni-hannover.de/mosaik/wiki
PALM/PALM-4U web page: https://palm.muk.uni-hannover.de/trac
KPP web page: http://people.cs.vt.edu/asandu/Software/Kpp
Jöckel et al., 2010, *Geoscience Model Development, 3, 717–752*
Kurppa et al., 2019, *Geoscience Model Development. 12, 1403–1422*
Maronga et al., 2019, *Meteorologische Zeitschrift, 28, 105 – 119*
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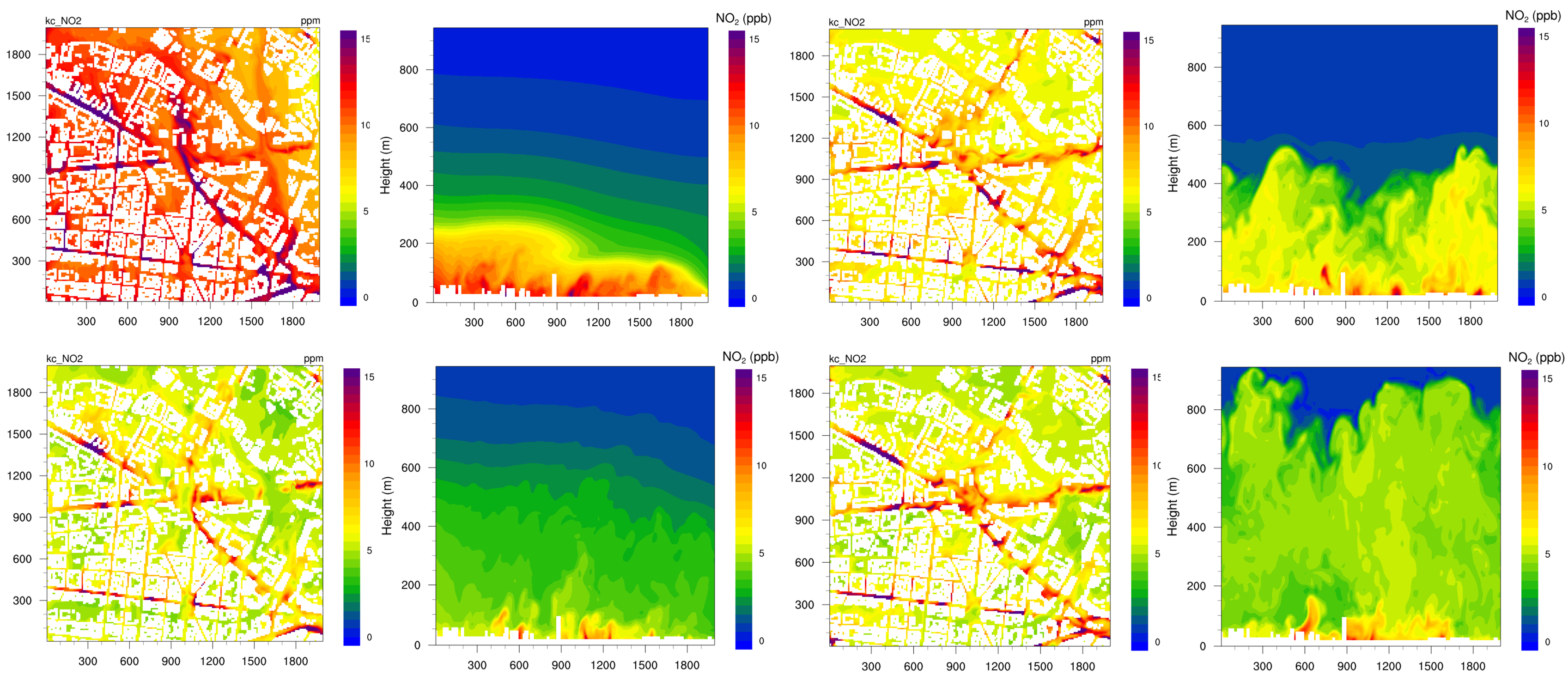
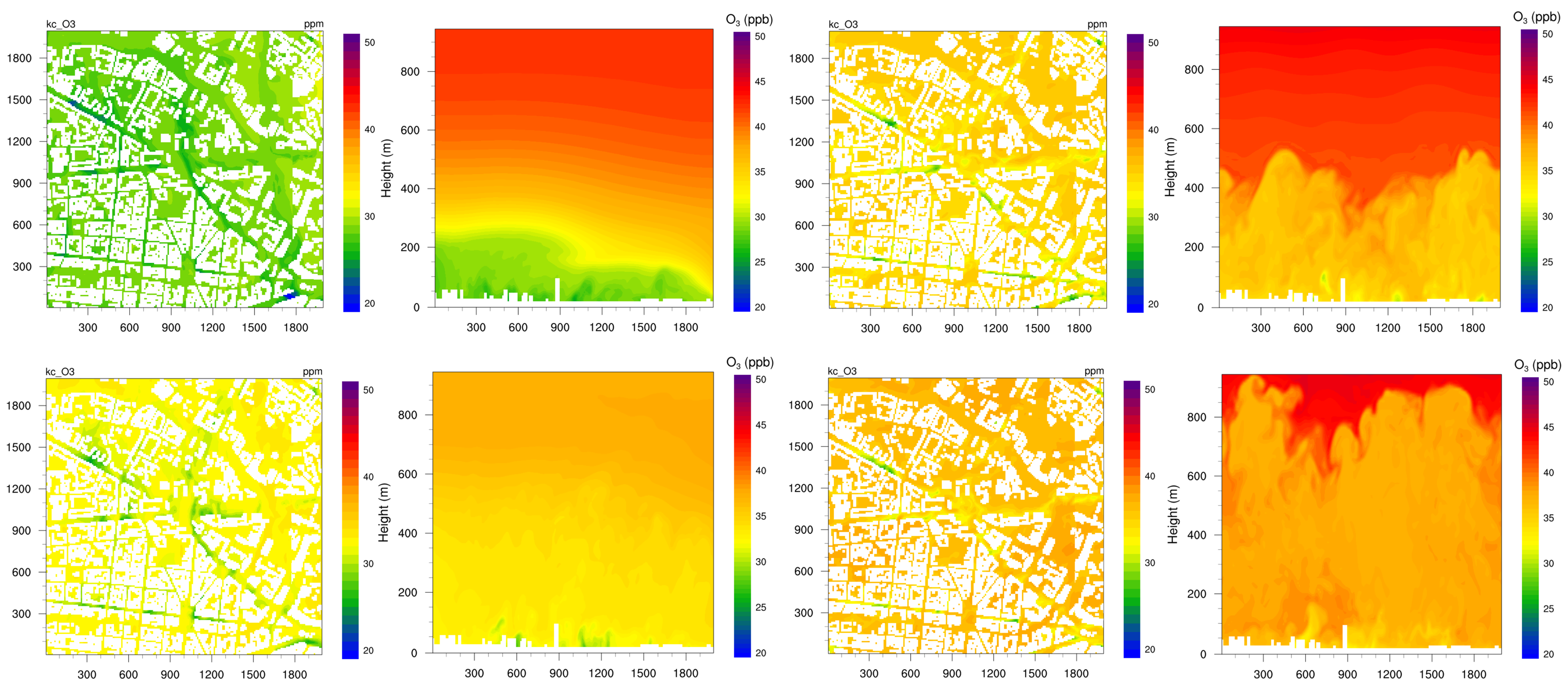
Saunders et al., 2003, *Atmospheric Chemistry and Physics 3, 161–180*

Results for different boundary conditions

Nested, BCs from WRF-Chem | **Cyclic boundary conditions**



NO_2 concentrations on July 29 2017, 8 CEST (top) and 9:30 CEST (bottom) with boundary conditions from WRF-Chem (left) and cyclic boundary conditions (right).



Same as above, but for ozone. All figures show instantaneous values. Horizontal cross sections are 5 m above ground, vertical cross sections are at y = 1000 m .

Although the observed near surface concentrations of ozone and NO_x were reasonably reproduced for both simulations, there was an improvement of the diurnal course when boundary conditions from WRF-Chem were applied instead of cyclic boundary conditions.

The use of cyclic boundary conditions results in a faster growth of the boundary layer during the morning and the height is overestimated by 10 to 15% whereas the boundary layer top is not sufficiently distinct with 'offline nesting' into WRF-Chem.

Turbulent fluctuations, which are needed as boundary conditions for the LES model are not provided by regional models. To compensate for the lack of turbulent velocity components in output of regional models small scale turbulence is imposed by a turbulence generator if PALM-4U receives boundary conditions from a mesoscale model. Since large eddies a not created by the turbulence generator is, the extension of the current test domain is not sufficient to obtain fully developed turbulence. A test simulation with offline nesting into COSMO without chemistry indicates that it takes up to 5 km until larger eddies are developing.

Concluding remarks

PALM-4U is able to simulate resolved turbulent transport and chemical transformations in the urban environment at very high resolutions – also for more complex chemical mechanisms than shown here.

This preliminary implementation of lateral boundary values of mean quantities from a mesoscale simulation with WRF-Chem allows to consider the effect of regional pollutant transport and improves the quality of chemistry simulations with PALM-4U. However, very large domains are required so far for a good representation of the turbulence in the boundary layer.

PALM-4U is under further development, which includes – among others – also the use of boundary conditions for chemistry and their final inclusion in the preprocessor.

Acknowledgement

MOSAIK is funded by the BMBF (German Federal Ministry of Education and Research) under grant 01LP1601 within the framework of Research for Sustainable Development (FONA; www.fona.de)

GEFÖRDERT VOM Bundesministerium für Bildung und Forschung

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