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

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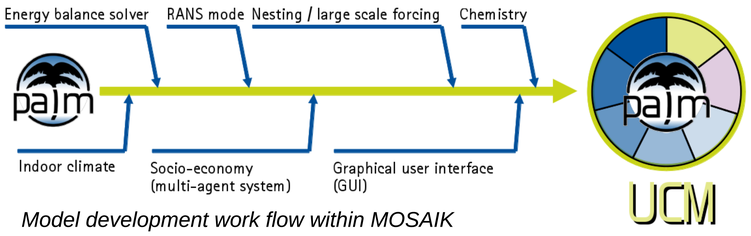
Introduction

Adequate modelling tools are required to support urban planning and the development of strategies aiming at minimizing adverse effects on urban climate such as poor air quality. However, a realistic implementation of urban canopy processes still poses a serious challenge for current weather and air quality models due to the small scale of the phenomena to be described.

To address this demand, a new microscale urban climate model (UCM) is developed within the joint project **MOSAIK** (**Mo**dellbasierte **S**tadtplanung und **A**nwendung **i**m **K**limawandel: Model-based city planning and application in climate change, https://palm.muk.uni-hannover.de/mosaik/wiki) under the lead of the Institute of Meteorology and Climatology at the Leibniz Universität Hannover.

The new urban climate model **PALM-4U** is based on the state-of-the-art **Pa**rallelized **L**arge-Eddy Simulation **M**odel (PALM, Maronga et al, 2015). In addition to atmospheric chemistry, PALM-4U will also include modules for indoor climate and energy demand and human-related quantities (physiological equivalent temperature or universal thermal climate index) in its final stage and will be coupled to a multi-agent model.



Model development work flow within MOSAIK

Chemistry implementation LES Model PALM-4U

A fully coupled 'online' chemistry model has been implemented into PALM-4U. Automatic generation of the chemistry code with the Kinetic Pre-Processor (KPP, Damian et al., 2002) and KP4 (Jöckel et al., 2010) allows for high flexibility in the choice of gas phase chemical mechanisms of different complexity.

Due to the high computational demands of LES, compromises are necessary with respect to the degree of detail of the atmospheric chemistry. A simulation for the entire city of Berlin with 10 m grid width and 4704x3920x336 grid points and two nested sub-domains with 2 m grid width is planned as part of the MOSAIK project, which will already require a huge amount of CPU time even without chemistry. Therefore, chemistry mechanisms with 30 to 100 reactions and up to 200 chemical compounds, which are usually applied with regional models are not applicable with LES models over large model domains.

Currently PALM-4U includes the following chemistry options:

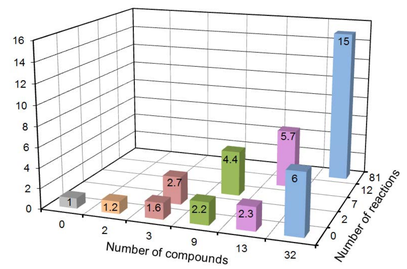
- **CBM4** (Carbon Bond Mechanism, Gery et al. 1989, 32 compounds, 81 reactions)
- **SMOG** (a simple photochemical smog mechanism, 13 compounds, 12 reactions)
- **SIMPLE** (further simplification of SMOG, 9 compounds, 7 reactions)
- **PHSTAT** (photo-stationary state only, 3 compounds, 2 reactions)
- **PASSIVE** (just 2 passive tracers, no chemical reactions)

Test of chemistry module performance in PALM-U

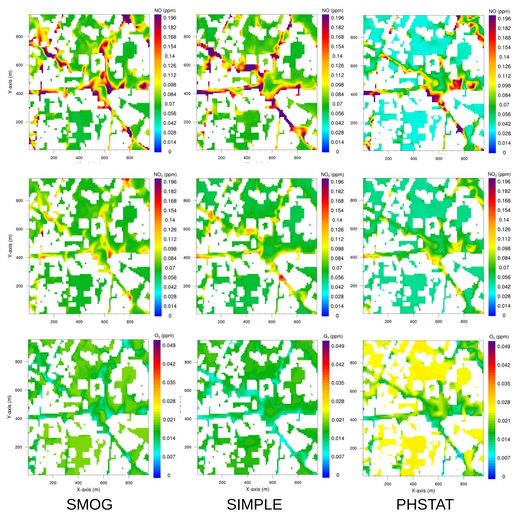
Test simulations with PALM-4U were performed with the chemistry mechanisms CBM4, SMOG, SIMPLE and PHSTAT, and also with the module describing just two passive tracers. The test simulations were carried out for a model domain with 96x96 points and 10 m grid width. The domain covers a small area of Berlin around the Ernst-Reuter-Platz, a junction with some high buildings and heavy car traffic.

Since detailed emission data are not yet available, only traffic emissions, which were parameterized depending on the street type classes from OpenStreetMap were considered

Due to the random nature of turbulence, instantaneous values of pollutant concentrations show local differences. However, on the average concentration fields of NO, NO_2 and ozone are comparable for the different mechanisms except for the photo-stationary equilibrium.



CPU time requirement of 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 mechanisms' compounds is considered.



Concentrations of NO, NO_2, and ozone at 10 UTC

Outlook

PALM-4U is still under extensive development, which also holds for its chemistry module. More mechanisms will be added and already implemented mechanisms undergo further testing. The optimum mechanism will however depend on the field of application. Efforts will be made to speed up chemistry (vector version, larger time steps for chemistry). Furthermore, an implementation of the SALSA aerosol module (Kokkola et al, 2008) was coupled to the gas phase chemistry and is currently tested.

References:
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