Development of an online chemistry model for the microscale urban climate model PALM-4U within the [UC]$^2$ programme

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[UC]$^2$: Project structure

- **Urban Climate Under Change [UC]$^2$:** Research project funded by the German Federal Ministry of Education and Research (BMBF), 2016-2019

- **Goal:** Development of a new (building resolving) urban climate model for scientific research and applied urban planning → PALM-4U (= PALM for urban applications)

![Diagram showing project structure]

- **Module A:** Model development
  - MOSAIK

- **Module B:** Observations & wind tunnel
  - 3DO

- **Module C:** Practicability & user-friendliness
  - UseUClim/KliMoPrax
[UC]$^2$: Project structure

Module A
- Model development
  - Model validation
  - Users in science and practise
    - Applicability tests
Module B
- Observational data
  - Applicability tests
Module C
- Practicability and usability
  - Applicability tests

IOP I
- Winter 2017
IOP II
- Summer 2017
IOP III
- Winter 2018
IOP IV
- Summer 2018
[UC]$^2$: Project structure

### [UC]$^2$ Publications

**Scherer et al., 2019:** Urban Climate Under Change [UC]$^2$ – A National Research Programme for Developing a Building-Resolving Atmospheric Model for Entire City Regions
DOI: 10.1127/metz/2019/0913

**Maronga et al., 2019:** Development of a new urban climate model based on the model PALM – Project overview, planned work, and first achievements
DOI: 10.1127/metz/2019/0909

**Scherer et al., 2019:** Three-Dimensional Observation of Atmospheric Processes in Cities
DOI: 10.1127/metz/2019/0911

**Halbig et al., 2019:** Urban Climate Under Change – Module C of the Research Programme: User Requirements and Case Studies to Evaluate the Practicability and Usability of the Urban Climate Model PALM–4U.
Module A: From PALM to PALM-4U
Overview of capabilities

PALM: the model core (Maronga et al. 2015, GMD)
- Parallelized large-eddy simulation (LES) model
- Incompressible and anelastic
- Highly-optimized, high scalability
- Topography on Cartesian grid
- Embedded models

PALM-4U: PALM + additional components

Energy balance solver  RANS mode  Nesting / large scale forcing  Chemistry

Indoor climate  Socio-economy (multi-agent system)  Graphical user interface (GUI)
Processes in PALM-4U

**Urban Surfaces**
- Energy balance
- Heat conduction
- Solid materials
- Green elements

**Vegetation**
- Energy balance
- Sink for momentum
- Shading
- Roots
- Soil moisture

**Chemistry**
- Transport
- Chemical reactions
- Photolysis
- Emissions

**Radiation**
- Energy balance
- Shading
- Reflections

**Impact**
- Multi-agent system
- Biometeorological analysis
- Indoor climate

**Technical Solutions**
- Mesocale nesting
- LES-LES nesting
- RANS mode
- User-friendly GUI

Special Issue in GMD coming soon
Berlin showcase: Set-up

- 24h simulation (21/7/13), Start 0:00 MESZ
- 24h spinup: Surface and radiation
- „parent“ domain:
  Berlin (47 x 39 km$^2$ @ 10m resolution)
- „child“ domain:
  Government district (1 km$^2$ @ 1m res.)
- Forcing: COSMO-DE initial profiles, 21 July 2013 at midnight
- Synoptic situation: weak winds, clear sky, COSMO-DE near-surface temperatures of > 303 K
- Lateral boundaries: (from parent) cyclic

Resources:

parent:
4704*3920*336 grid points, 10.976 cores, 11 Tbyte memory

child:
1024*1024*320 grid points, 1.024 cores
1h real time ~ 15 h wall clock time
Berlin showcase: Air temperature

night time

0400 UTC

day time

1200 UTC

(K)
294.8
294.2
293.6
293.0
292.4
291.8
291.2
290.6
290.0
289.4
288.8

(K)
300.9
300.6
300.3
300.0
299.7
299.4
299.1
298.8
298.5
298.2

θ (K)
303.0
300.0
297.0
294.0
291.0
288.0
285.0

0 4 8 12 16 20 24

time (UTC)

rural

urban
Berlin showcase: Air temperature

night time

day time
Chemistry module (1)

• An 'online' chemistry model has been implemented into PALM-4U

• Gasphase chemistry

  • Automatic generation of chemistry code with the Kinetic Pre-Processor (KPP, Damian et al., 2002) allows for high flexibility in the choice of gas phase chemical mechanisms
  • Adaption for PALM-4U based on KP4 post-processor (Jöckel et al., 2010)
  • PALM-4U includes a set of chemistry mechanisms of different complexity

→ Complexity of mechanism chosen by user depending on application

→ Mechanisms can easily be added by user
Chemistry module (2)

CBM4: Carbon Bond Mechanism (Gery et al. 1989, 32 compounds, 81 reactions)
SMOG: Small photochemical mechanism (13 compounds, 12 reactions)
SIMPLE: Simplified of SMOG (9 compounds, 7 reactions)
PHSTAT: Photo-stationary state (3 compounds, 2 reactions)
PASSIVE: Two passive tracers (2 compounds, 0 reactions)
Reference: Meteorology only

Resources:
PALM-4U chemistry run using the different provided mechanisms
Chemistry module (3)

- A simple photolysis parameterization: Dependency on solar altitude and chemical component following Saunders et al. (2003)

- Try deposition following resistance approach
  - DEPAC module for gases (van Zanten et al., 2010)
  - Reactive and passive aerosols following Zhang et al. (2001)

- Coupled to the sectional aerosol module SALSA (Kokkola et al., 2008) which has been implemented into PALM
  → External contribution, Kurppa et al. 2019 (GMD)
Emission module:
Anthropogenic emissions can be provided in different levels of detail

(1) Via netcdf input as gridded data, temporally disaggregated or annual emission information

(2) Parameterised traffic emissions relying on the street type classes from OpenStreetMap and emission factors following HBEFA 3.3, input via namelist
Chemistry module – First results

- Berlin, Germany, Ernst-Reuter-Platz
- 10 m resolution, 1km x 1km x 3 km
- Parameterised traffic emissions relying on street type
- Small photochemical mechanism ‘SMOG’ (13 compounds, 12 reactions)
- Summer time simulation, 21st of July

Concentration of NO₂ in ppm (5m)

Z-Y-vertical cross section at dashed line: Concentration (shaded color) of NO₂ and O₃ in ppm and vertical velocity (-2.0 to 2.0 m s⁻¹, negative values as dashed lines)
Chemistry module – First results

- Berlin, Germany, Ernst-Reuter-Platz
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Animation!!!

Concentration of NO₂ in ppm (5m)  Z-Y-vertical cross section at dashed line: Concentration (shaded color) of NO₂ and O₃ in ppm and vertical velocity (-2.0 to 2.0 m s⁻¹, negative values as dashed lines)
Chemistry module – First results

Diurnal cycle

Profiles

09:00 CET

17:00 CET
Recognise the urban quarter below?

- Aerosol module SALSA coupled to PALM
- Implementation of SALSA and evaluation for a street-canyon (Pembroke Street) in central Cambridge → Kurppa et al., 2019 (GMD)
- 24 hours simulation @ 1m resolution on March 20–21, 2007 compared to measurements (Kumar et al., 2008, 2009)
- Parameterised emissions

**Total aerosol number concentration Ntot (m$^{-3}$)**

**Animation!!!**

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**Animation!!!**
Conclusions and Outlook

- Turbulence and building resolving LES model including chemistry, applicable for scales way beyond street canyon, up to city-scale

- PALM-4U → Future state-of-the-art urban climate model

- Further improvements and applications of chemistry module
  - Comparison to measurements, city-scale applications
  - Connection to multi agent module → pollutant exposure
  - Offline Nesting: Lateral boundary conditions from mesoscale atmospheric chemistry model
  - Inclusion of pollen
  - Enhanced aerosol description
  - Biogenic emissions
  - Parameterised emissions for emissions from residential heating and large point sources
  - Wet deposition
Thank you for your attention!

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http://palm4u.org

https://palm.muk.uni-hannover.de/mosaik/wiki

http://palm-model.org