Development and Application of an Online Coupled Chemistry Urban Microscale Model PALM-4U

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OUTLINE

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BACKGROUND

- The MOSAIK Project
  The German Federal Ministry of Education and Research (BMBF), funded a joint project in 2016, named as Model-based city planning and application in climate change (MOSAIK) to develop an urban climate model within the framework of Urban Climate Under Change ([UC]²).

- Main Aim
  To develop a highly-efficient, state-of-the-art high-resolution microscale urban climate model that allows for building and turbulence-resolving simulations of large cities such as Berlin (Germany).

- PALM, the core Model
  PALM (Raasch and Schröter, 2001; Maronga et al., 2015) was selected as the core model for the new microscale UC model named as PALM-4U of large cities such as Berlin (Germany).

1995: Prof. Siegfried Raasch! After his first successful PALM LES run.
The PALM is based on the non-hydrostatic, filtered, incompressible Navier-Stokes equations in Boussinesq-approximated form.

The Model has 6 prognostic quantities (u, v, w, θ, q_v and an optional ‘s’ for passive tracer).

An additional equation for subgrid scale TKE ‘e’ (default LES mode) OR The total TKE (RANS mode).
PALM-4U = PALM-LES + Urban Climatology + Air Chemistry

- Multiagent Model
- Indoor Climate
- Human Bio-meteorology
- Urban Canopy Model
- Radiative Transfer in Urban Canopy
- Chemistry Model
- PALM Dynamic Core
PALM-4U! A Microscale Urban Climate & Air Quality Model
Interface b/w Chemistry and PALM-4U

Chemistry Driver

- Deposition, Emission, Emission inventory (anthropogenic and biogenic*).
- Lateral BC's

Chemistry Driver

- KP4 Pre-processor
- Processes and reorganizes KPP output to generate code for palm-4u

Chem_gasphase_mod.f90
- Chem spcs defined
- Contains integration and rosenbrock calc. subroutines.

Aerosol Chemistry (SIA and SOA)*

KPP
- Kinetic Pre-processor (x) for Chem Spcs.
- Chem Mechanisms are defined here.

PALM-4U - LES

* Not implemented as yet

(x) Damian et al., 2002
http://people.cs.vt.edu/asandu/Software/Kpp/
Current Features of Chemistry Model in PALM-4U Modeling System:

- An ‘Online’ coupled chemistry in LES mode for Gas-phase chemistry.
- Chemical reactions,
- Advection and diffusion
- Photolysis
- Ability to take any user provided chemical mechanism
- Passive tracer
- Nesting
- Static emissions in time and space.
A Case Study from Downtown Berlin - Germany

Model Setup

- \( n_X = n_Y = 96, n_Z = 120; d_X = d_Y = d_Z = 10 \text{ m}; U_g = V_g = 1.0 \text{ m s}^{-1} \)
- Day & Time: 21 July, 5:00 UTC; Simulation length = 6 hours.
- Modules: radiation, urban surface model, land surface model, canopy model, chemistry model, photolysis model
- Emissions related to OpenStreetmap street types:
  Enhancement factor for main roads = 0.1667, Reduction factor for side roads = 0.334
- Emission: \( \text{NO} = 1.318 \text{ ppm s}^{-1}; \text{NO}_2 = 0.368 \text{ ppm s}^{-1}; \text{RH} = 0.1804 \text{ ppm s}^{-1}; \text{PM10} = 0.75 \text{ug m}^2 \text{s}^{-1} \).

The mechanism has 11 gas-phase chemical species and one non-reactive aerosol (PM10).

1. \( \text{NO}_2 + h\nu = \text{NO} + \text{O}_3 \)  : photon(j_no2)
2. \( \text{O}_3 + h\nu = 2\text{OH} + \text{O}_2 \)  : photon(j_o31d)
3. \( \text{NO} + \text{O}_3 = \text{NO}_2 \)  : arr2(1.8E-12_dp, 1370.0_dp, temp)
4. \( \text{RH} + \text{OH} = \text{RO}_2 + \text{H}_2\text{O} \)  : arr2(2.E-11_dp, 500.0_dp, temp)
5. \( \text{RO}_2 + \text{NO} = \text{NO}_2 + \text{RCHO} + \text{HO}_2 \)  : arr2(4.2E-12_dp, -180.0_dp, temp)
6. \( \text{HO}_2 + \text{NO} = \text{NO}_2 + \text{OH} \)  : arr2(3.7E-12_dp, -240.0_dp, temp)
7. \( \text{NO}_2 + \text{OH} = \text{HNO}_3 \)  : arr2(1.15E-11_dp, 0.0_dp, temp)
8. \( \text{PM10} = \text{PM10} \)  : 1.0_dp
Results

Time series plot of trace gases and passive tracer PM10

- PM10
- RH
- O3
- NO
- NO2

[Graph showing time series data with various trace gases and PM10 concentrations]
Results

[a Case Study-Berlin]
Results

[A Case Study-Berlin]
Results

Horizontal cross-sections; Level: 5 meter; Left Panel: NO₂ shaded, W-Contours, Right Panel: O₃ shaded and horizontal wind vectors.

Time Label : 30 minutes.
Results

Vertical cross-sections; **Left Panel**: NO$_2$ shaded, W-Contours,
**Right Panel**: O$_3$ shaded, potential temperature contours.

Vertical Velocity Contours -2:+2 m s$^{-1}$

Potential Temp Contours 282: 300 K
Summary and Outlook

Summary

- Turbulence and building resolving LES PALM-4U model allows accurate simulation of advection, reaction, and deposition of atmospheric trace gases and aerosols at appropriate scale.
- PALM-4U is a potential candidate for the future state-of-the-art comprehensive urban climate modelling system that could be used for the assessment, prediction and investigation of urban climatology, air quality and city planning of large urban areas.

Coming soon …

- Chemistry forcing at the lateral boundaries of the parent domain
- Aerosol chemistry (SIA and SOA). SALSA sectional aerosol model (Kokkola et al., 2008) in the process to be incorporated in PALM-4U.
- Deposition module for chemical species and aerosols.
- Detailed anthropogenic emissions (temporal and spatial disaggregation, VOC split etc.).
- Reynolds Averaged, Navier-Stokes (RANS) Mode for larger domain, longer simulations and complex mechanisms.
Wenn du Luft atest, solltest Du Dich darum kümmern!

Danke für die Aufmerksamkeit!

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