The PALM chemistry model

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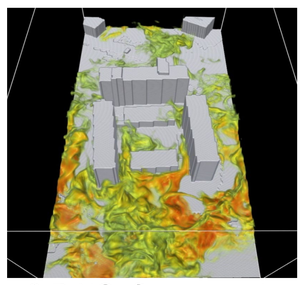
Features and set-up of the PALM chemistry model

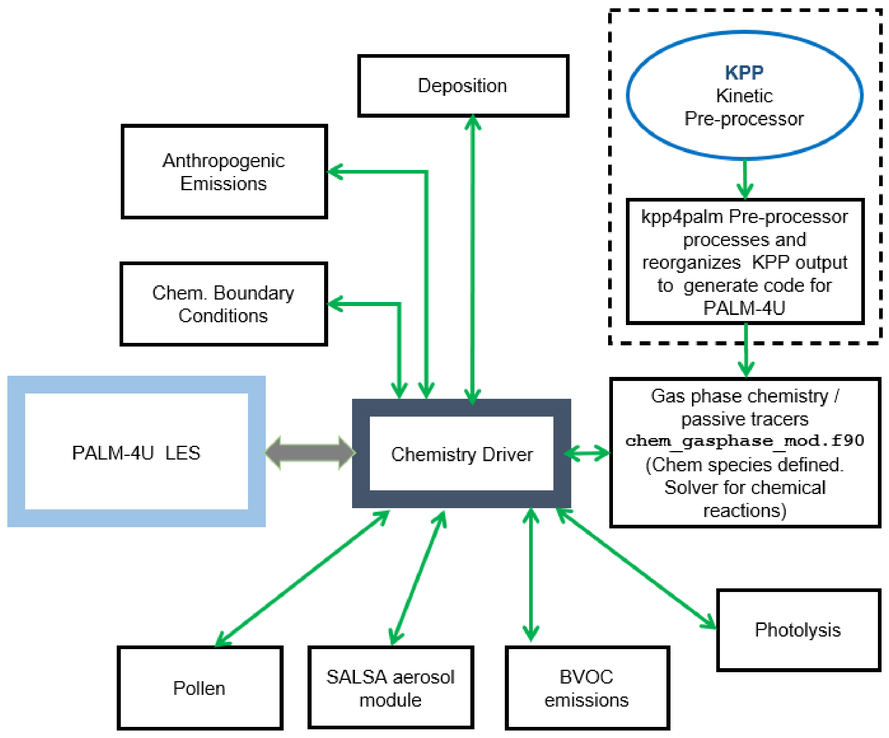
The chemistry model is coupled 'online' into PALM which implies that the prognostic equations for the chemistry compounds are solved consistently with the equations for momentum, heat, and water constituents. The current features of the chemistry model are:

- Flexible gas-phase chemistry implementation based on the **K**inetic **P**re-**P**rocessor (KPP)
  - Fortran subroutines solving rate equations of given gas phase chemistry mechanism are generated automatically
  - PALM includes a number of ready-to-use chemical mechanisms
- Photolysis calculation including shading effects
- Dry deposition
- Anthropogenic emissions (as surface fluxes and point sources)
- Biogenic VOC emissions
- Pollen emissions
- Aerosol: Passive tracer, ISORROPIA, SALSA

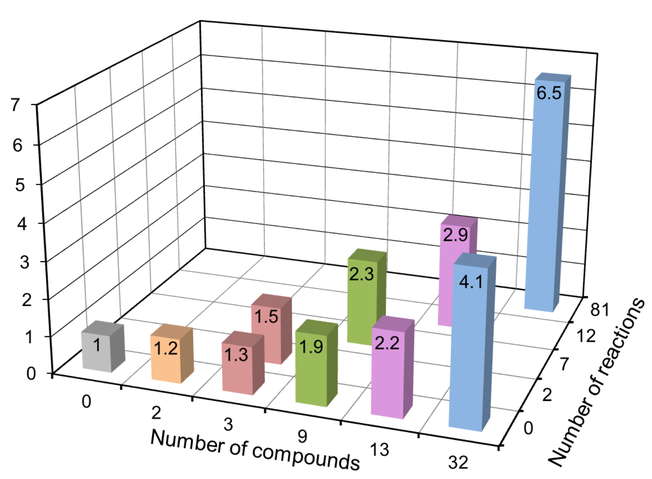


3-D NO_2 flow around buildings

The chemistry code is structured as shown in the figure on the right hand side. The KPP preprocessor for the gas-phase chemistry implementation is the starting point which is creating the corresponding code that is then converted to a PALM subroutine by the kpp4palm pre-processor. This subroutine (chem_gasphase_mod.f90) is then called by the chemistry driver of PALM which handles all available chemistry modules. It calls the photolysis module, the emission module etc. and other connected modules, and is also handling the chemical boundary conditions.



Computational demand: Ready-to-use mechanisms

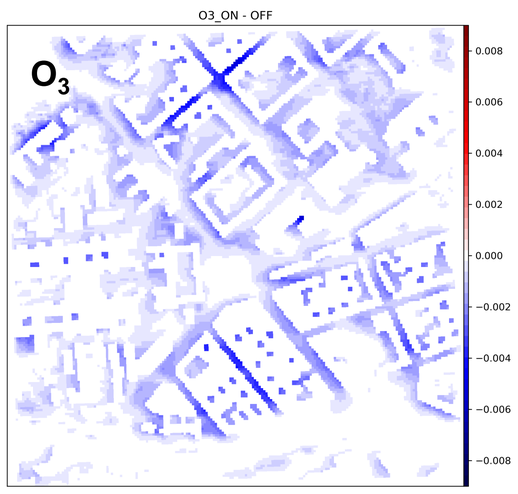


Resources required for PALM-4U chemistry run (test for one day with Intel compiler for 96 x 96 x 320 grid points)

CPU time requirement for a PALM run using the different provided mechanisms relative to a meteorology only run (grey bar):

- **CBM4**: Carbon Bond Mechanism (Gery et al. 1989, 32 compounds, 81 reactions)
- **SMOG**: Small photochemical mechanism (13 compounds, 12 reactions)
- **SIMPLE**: Simplified version 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

Building Shadow Effects



Simulation for a 1x1 km² area in Berlin with the CBM4 chemical mechanism.

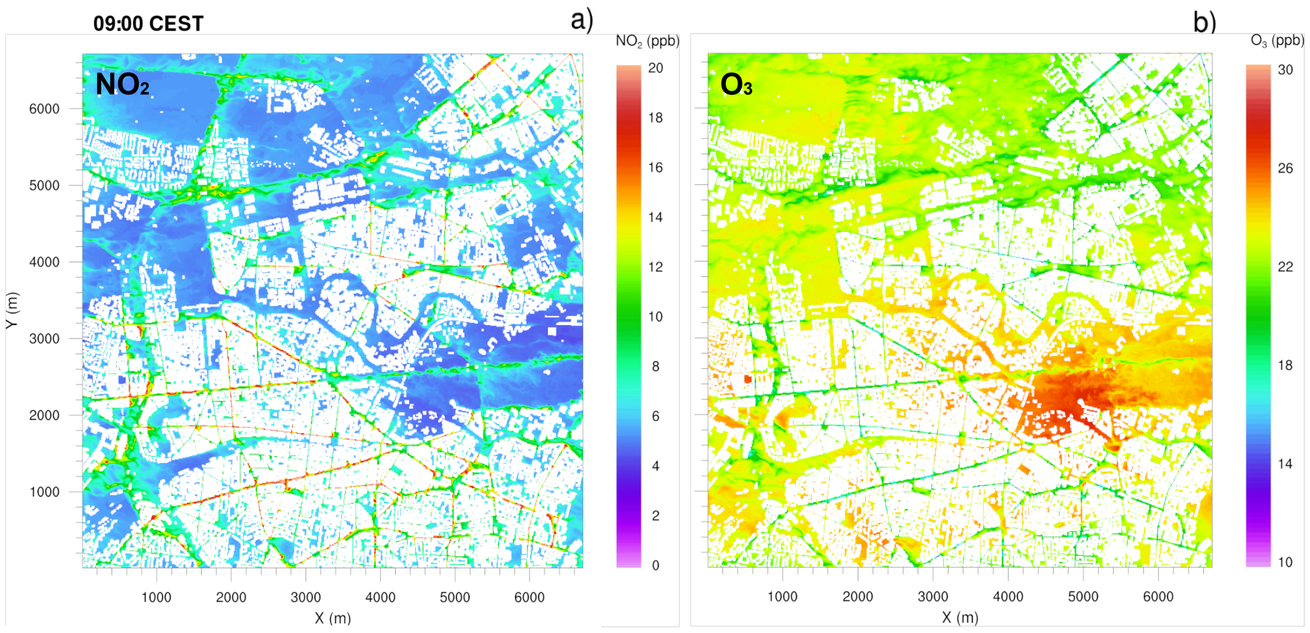
- Less near surface O_3 and NO, more NO_2 for low sun elevation
- On the average 5% to 10% relative difference (absolute concentration differences are usually quite small) in the morning and evening hours.
- Almost no differences around noon
- Mixing leads to shadow effects also above the buildings

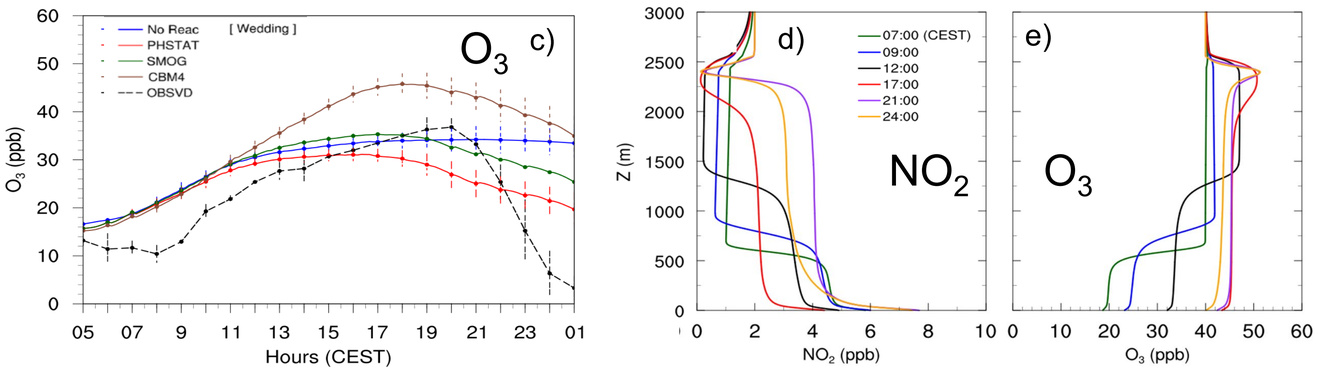
Difference in near surface O3 concentration between simulation with and without shadow effect at 12:30 h.

A case study for Berlin

The fully coupled chemistry online microscale PALM model was employed to simulate gas-phase photochemistry on a summer day in Berlin (Khan et al., 2021). The CBM4 chemistry mechanism has been used. Plots (a & b) show the spatial distribution of the concentrations of NO_2 and O_3.

- Only parameterized traffic emissions are included
- High NO_2 levels over the road network in the middle to sourthern part of the domain due to high NO emissions and excessive O_3 titration.
- High O_3 levels in the less urbanised area of Tiergarten and the northern part of the domain due to lower NO emissions.
- Vertical profiles (d and e) show mixing and chemical transformation of chemical species over the diurnal cycle



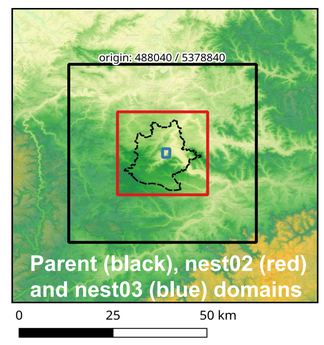


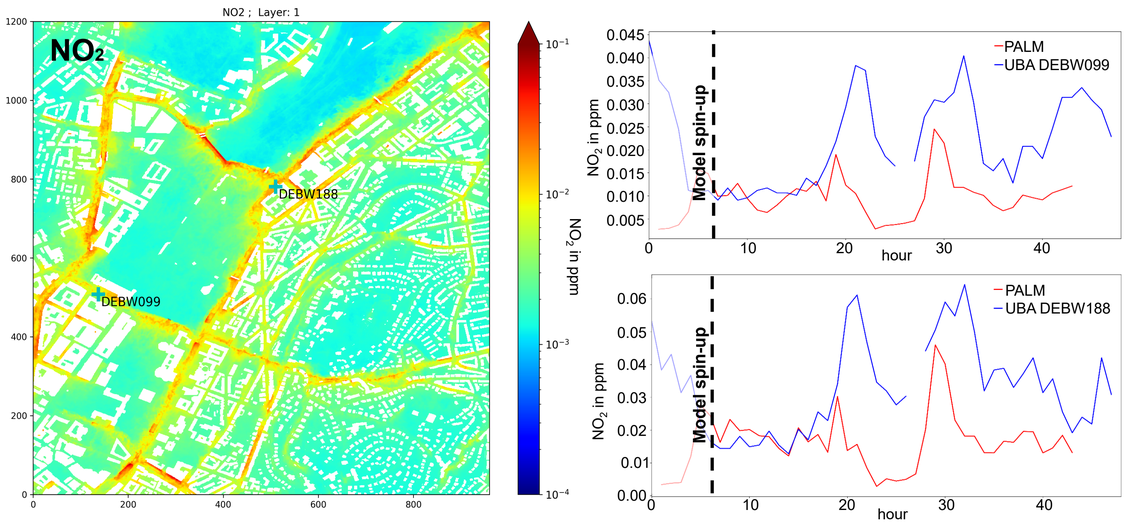
Comparison to observations from Hardenbergplatz using three different mechanisms

Vertical profiles of NO_2 and O_3 at different times of the day

Model validation run for Stuttgart (VALM04)

- City-wide run from 8th to 9th of July 2018 with parent domain (Δx:40m), nest02 (Δx: 10m) and nest03 (Δx: 2m)
- Offline-nesting with COSMO-Model
- Chemical boundaries from WRF-Chem
- Emission input (as LOD 2 surface fluxes)
  - MATSim emissions for traffic sector (on 2x2 m²)
  - Data from University of Stuttgart, IER (D. Schmid, A. Altstadt), for further sectors including industrial and stationary combustion (on 1x1 km²)





Spatial distribution of modelled NO_2 concentrations (left panel) in nest03 at 10:00 UTC and time series of modelled (red) and observed (blue) NO_2 concentrations at stations Stuttgart Neckartor (DEBW188) and Stuttgart Anulf-Klett-Platz (DEBW099)

- Highest NO_2 concentrations on/close to streets
  - Traffic is the main emission source
- Modelled concentrations follow course of observed concentrations
  - Shifts in time partly due to modelled work day versus weekend as July 8th 2018 was a Sunday
- Modelled concentrations lower than observed concentrations
  - Emissions underestimated/missing sectors in emission input
  - Dispersion limited due to numerical issues with emission input as line information

Reference:
Khan, B. A., Banzhaf, S., Chan, E. C., Forkel, R., Kanani-Sühring, F., Ketelsen, K., Kurppa, M., Maronga, B., Mauder, M., Raasch, S., Russo, E., Schaap, M., and Sühring, M. (2021). *Development of an atmospheric chemistry model coupled to the PALM model system 6.0: impelementation and first applications, Geoscientific Model Development, 14, 1171–1193.*

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