E5 – Chemistry modelling for an urban area with traffic emissions

Institute of Meteorology and Climate Research
Atmospheric Environmental Research
Campus Alpin

Karlsruhe Institute of Technology

Institute of Meteorology
Tropospheric Environmental Research
Freie Universität Berlin

Freie Universität Berlin

Klaus Ketelsen, Software developer

Description

This exercise is about using the chemistry model. The aim is to learn:

- how to switch on chemistry
- about the main chemistry options
- how to apply different chemistry mechanisms
- how to apply different options for anthropogenic emissions

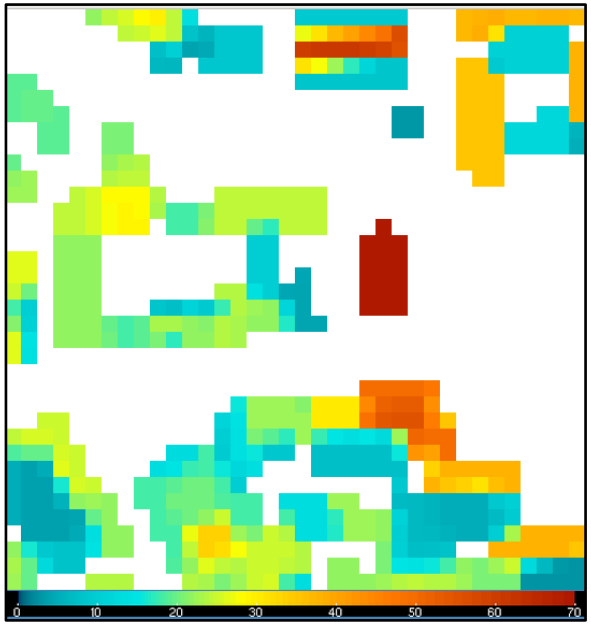
Requirements

- Lecture „Chemistry model“
- Lecture „Static and dynamic drivers“

Summary of simulation setup

General setup

- Small part of Berlin with realistic distribution of streets and buildings
- 10 m grid width
- Cyclic boundary conditions
- Short runs for instationary conditions around sunrise
- **Baseline** run for **photostationary equilibrium** between NO, NO_2 and O_3 plus one passive tracer and parameterized traffic emissions



Building heights from the static file for this exercise

Note that the quality of the results is limited due to the small size of the model domain and the coarse resolution (mainly a meteorology issue – the chemistry will run stable nevertheless).

Input files to start with the excercise are supplied in:
E-5_chemistry_steering_files_incomplete.zip

General setup

Input files to start with the excercise are supplied in
=> **E-5_chemistry_steering_files_incomplete.zip**

Containing files:

- **`chem_phstatp_p3d`** (p3d with simple chemistry namelist for phstatp mechanism)
- **`chem_phstatp_static`** (static file for the area shown on the slide before)
- **`chem_phstatp_lod2_chemistry`** (time dependent traffic emissions for Task 3)

For completeness, the directory structure including the ready-to run files for the exercise are supplied in E-5_chemistry_steering_files_complete.zip.

Please do not look into E-5_chemistry_steering_files_complete.zip before you tried to solve the exercise yourself!

Task 1: Simulation with the phstatp mechanism from 06 UTC to 08 UTC (baseline case)

- **Simulation time**: 06 to 08 UTC
- **Mechanism:** photostationary equilibrium between NO, NO_2 and O_3 plus one passive tracer named PM10 (mechanism **phstatp**)
- **Emissions:** parameterized traffic emissions (**`emiss_lod = 0`**)

Create and run a simulation setup named `chem_phstatp`

1. Create a simulation setup **`chem_phstatp`** in the **`JOBS`** directory.
   Hint: Use the input files **`chem_phstatp_p3d`** and **`chem_phstatp_static`** supplied in **`E-5_chemistry_steering_files.zip`**
2. Run your setup for **`chem_phstatp`**
3. Look into the results

Preliminary question

(1) Where can I expect high traffic emissions in my domain?
Hint: What is the meaning of `emiss_lod = 0`?
Look into the static file

Question on simulation results

(View results with ncview or a similar simple viewer - with ncview, you can get time series by clicking at a point)

How do the concentrations of PM10, NO, NO_2 and ozone correlate?
Look at area plots at the end of the simulation and at time series for ozone, NO and NO2, and PM10 at x=285m and y=185m.

Task 2: Simulation with the smog mechanism from 06 UTC to 08 UTC

Create and run a simulation setup with run_identifier named `chem_smog`

1. Use **`chem_phstatp_p3d`** as a basis for your namelist file **`chem_smog_p3d`** and use the same static file as in Task 1
   Hint: Preferrably use a soft link to obtain **`chem_smog_static`** instead of copying the static file into **`chem_smog`**

2. Create a **`USER_CODE`** directory in **`JOBS/chem_smog`** and add **`chem_gasphase_mod.f90`** for smog into this directory
   Hint: Look into **`packages/chemistry/kpp4palm/mechanisms`**

Create and run a simulation setup named `chem_smog` (cont.)

3. Edit your **`chem_smog_p3d`**

   a. Include parameterized surface emissions (**`surface_csflux`**) to the namelist for RH (649 μmol m^{-2} d^{-1}), RCHO (30 μmol m^{-2} d^{-1}), and CO (30000 μmol m^{-2} d^{-1})
   Hint1: smog does not conclude PM10
   Hint2: Do not forget to extend the number of factors for **`emiss_factor_main/side`** by the number of new variables.

   b. Additional initial values/profiles:
   RH: linear decrease of 0.010 ppm at surface to 0.005 ppm at 295 m, constant above
   RCHO: same profile as for RH, but only half of the concentration of RH
   CO: 0.1 ppm at all heights

   c. Add instantaneous 3d output for the three new initialized variables (RH, RCHO, CO) and for concentrations of OH, HO2 and HNO3

Create and run a simulation setup named `chem_smog` (cont.)

4. Start a simulation with your setup chem_smog
   (Will take much longer than for phstatp. If the simulation takes too long, re-run the simulation for a shorter time)

5. Analyze results e.g. with ncview.

   - Compare and explain the differences in the concentrations of ozone for phstatp and smog at 5 m above the ground (at 7200 sec if available or for an earlier time).

   - Look at time series for ozone, NO2 and NO, products and radicals at x=285m and y=185m at a height of 5 m.

Preliminary questions

(1) Where can we find the **`chem_gasphase_mod.f90`** for smog?

(2) What about PM10 when running PALM with smog? Keep or remove? How can we find out?
Hint: Check either **`chem_gasphase_mod.f90`** or the .eqn file in the respective subdirectory of **`packages/chemistry/kpp4palm/mechanisms`**

Question on simulation results

Why is ozone higher for smog than for phstatp?

Hint: Check either **`chem_gasphase_mod.f90`** or the .eqn file in the respective subdirectory of **`packages/chemistry/kpp4palm/mechanisms`**

Task 3: Run with LOD 2 emission input and phstatp mechanism

Create and run a simulation setup named `chem_phstatp_lod2`

- Create the simulation setup **`chem_ phstatp_lod2`** by adapting **`chem_phstatp_p3d`** concerning the emission input (LOD 2 instead of LOD 0)
- Remove namelist parameters that are only needed for the parameterized emissions of LOD 0 (**`surface_csflux*, *street*)`**
- Use the same static file as in Task 1 and Task 2 and copy the chemistry driver **`chem_phstatp_chemistry,`** which contains the pre-processed real-time traffic emissions to the INPUT directory (details on LOD 2 emissions are on next slide)
- Run the new setup and compare it to the results of **`chem_phstatp`**.
- Analyze the concentration results using ncview

Chemistry model exercise

Exercise Task 3

Short description of LOD 0 daily traffic emission values and LOD 2 traffic emission estimate

- **LOD 0**
  - Estimate using HBEFA 3.3 emission factors for exhaust emissions and mean traffic counts for Berlin differing main and side roads only. Temporal disaggregation based on a fixed week-day standard urban time profile
  - Main and side roads identified using the street_type classification from OpenStreetMap
  - For PM10 only emissions of car exhaust are considered. **No particle resuspension processes are taken into account!**
- **LOD 2**
  - Data based on calculations applying an emission model
  - Using HBEFA 3.3 emission factors (INFRAS, 2017) and hourly real-time traffic counts, temperature time series and the most current car fleet estimate for Berlin
  - **PM10 emissions include also emissions from particle resuspension** by using a corresponding parameterization for this emission source

Questions Task 3

Preliminary question

Take a look at the emission fields within the chemistry driver `chem_phstatp_lod2_chemistry` using e.g. ncview.
What is eye-catching when looking into the data?

Hint: Change “Axes“ and adapt the „Range“ in ncview to see the emissions of the different compounds (i.e. NO, NO_2 and PM10). Check „`emission_name`“ in the nc file using „ncdump“ to identify the different compounds (`ncdump -v emission_name chem_phstatp_lod2_chemistry`)

Question on simulation results

How much do the results using LOD 2 emission input differ from those of Task 1? Can you explain the differences in PM10 based on the description of the different emission inputs?

HINT: See previous slide and the description for the different LODs on https://palm.muk.uni-hannover.de/trac/wiki/doc/app/chememi or in the PALM model system on GitLab under:
palm_model_system-v23.04\packages\palm\model\docs\content\Guide\Modules\Chemistry

Chemistry model exercise

How to start

- Create INPUT directories for the different runs:
  - **`cd ~/palm/current_version`**

Task 1

- **`mkdir -p JOBS/chem_phstatp/INPUT`** : mechanism#1 run

Task 2

- **`mkdir -p JOBS/chem_smog/INPUT`** : mechanism#2 run
- **`mkdir -p JOBS/chem_smog/USER_CODE`**

Task 3

- **`mkdir -p JOBS/chem_phstatp_lod2/INPUT`** : mechanism#1 run with LOD2 emissions

Chemistry model exercise

How to proceed (Task 1)

Task1

- Copy **`chem_phstatp_p3d`** and **`chem_phstat_static`** to **`JOBS/chem_phstatp/INPUT`**
- **`palmrun -r chem_phstatp -X4 -T4 -a "d3#"`**

Analyze results in `JOBS/chem_phstatp/OUTPUT/chem_phstatp_3d.nc`

- **`ncview JOBS/chem_phstatp/OUTPUT/chem_phstatp_3d.nc &`**

  Create time series for a point by clicking on the 2d picture at this point

Chemistry model exercise

How to proceed (Task 2)

TASK 2

- **`cp JOBS/chem_phstatp/INPUT/chem_phstatp_p3d JOBS/chem_smog/INPUT/chem_smog_p3d`**
- **`cd JOBS/chem_smog/INPUT`**
- Create link to **`chem_phstatp_static`**, e.g.
  `ln -s ../../chem_phstatp/INPUT/chem_phstatp_static chem_smog_static`
- Copy **`packages/chemistry/kpp4palm/mechanisms/def_smog/chem_gaspase_mod.f90`** to **`JOBS/chem_smog/USER_CODE`**

- Edit **`chem_smog_p3d`**:

1. Add output variables

```
 data_output = 'theta', 'q', 'u', 'v', 'w', 'e',
…
'kc_NO2','kc_O3','kc_NO','kc_RH','kc_RCHO','kc_CO',
'kc_OH','kc_HO2','kc_HNO3',
. . .
```

2. Adapt mechanism name

```
chem_mechanism              = "smog",
```

Chemistry model exercise

How to proceed (Task 2, cont.)

- Edit **`chem_smog_p3d`** (cont):

3. Add/modify parameterized emissions

```
surface_csflux_name     = 'NO',   'NO2', 'RH', 'RCHO',  'CO',
surface_csflux          = 4745.0, 1326.0, 649.0, 30.0, 30000.0,   !
emiss_factor_main       = 1.667, 1.667, 1.667,  1.667, 1.667,     !
emiss_factor_side       = 0.334, 0.334, 0.334,  0.334, 0.334,
```

4. Add/modify initial surface concentrations and profiles

```
cs_name                 = 'O3',  'NO',  'NO2',  'RH', 'RCHO', 'CO',
cs_surface              = 0.025, 0.000, 0.010, 0.010, 0.003,  0.10,

cs_profile(1,:)         = 0.025, 0.040, 0.050,
cs_profile(2,:)         = 0.000, 0.000
cs_profile(3,:)         = 0.010, 0.002,
cs_profile(4,:)         = 0.010, 0.005,
cs_profile(5,:)         = 0.005, 0.0025,

cs_heights(1,:)         =  0.0, 305.0, 495.0,
cs_heights(2,:)         =  0.0, 295.0,
cs_heights(3,:)         =  0.0, 295.0,
cs_heights(4,:)         =  0.0, 295.0,
cs_heights(5,:)         =  0.0, 295.0,
```

Chemistry model exercise

How to proceed (Task 2, cont.)

- Run PALM with smog for start time 0600 to 0800 UTC

```
palmrun -r chem_smog -X4 -T4 -a "d3#"
```

- Analyze results with ncview

Chemistry model exercise

How to proceed (Task 3)

- **`cp JOBS/chem_phstatp/INPUT/chem_phstatp_p3d JOBS/chem_phstatp_lod2/INPUT/chem_phstap_lod2_p3d`**
- **`cd JOBS/chem_phstatp_lod2/INPUT`**
- Create link to **`chem_phstatp_static`**, e.g.
  `ln -s ../../chem_phstatp/INPUT/chem_phstatp_static chem_phstatp_lod2_static`
- Copy **`chem_phstatp_lod2_chemistry`** into **`JOBS/chem_phstatp_lod2/INPUT`**
- Open **`chem_phstatp_lod2_chemistry`** with ncview to have a look at the the variable **`emission_values`**:
  `ncview JOBS/chem_phstatp_lod2/INPUT/chem_phstatp_lod2_chemistry &`
  - Change “**`Axes`**” to “y” and “x” to see horizontal cross section
  - Adapt ”**`Range`**” according to the current species to see and assess the emission data

Chemistry model exercise

How to proceed (Task 3, cont.)

- Edit **JOBS/chem_phstatp_lod2/INPUT/chem_phstatp_lod2_p3d**:
  - **emiss_lod = 2,**
  - Remove or comment all namelist parameter needed for LOD 0 only: i.e. **surface_csflux_name, surface_csflux, emiss_factor_main, emiss_factor_side, main_street_id, side_street_id and max_street_id**

- Perform **palmrun -r chem_phstatp_lod2 -X 4 -T 4 -a "d3#"**

How to proceed (Task 3, cont.)

- Analyze results in **`JOBS/chem_phstatp_lod2/OUTPUT/`** and compare to **`chem_phstatp`** in **`JOBS/chem_phstatp/OUTPUT/`** with ncview
  - Compare **`chem_phstatp_lod2_masked_M01.nc`** to **`chem_phstatp_masked_M01.nc`**
  - Compare **`chem_phstatp_lod2_3d.nc`** to **`chem_phstatp_3d.nc`** e.g.
    - ncview **`JOBS/chem_phstatp_lod2/OUTPUT/ chem_phstatp_3d.nc &`**
    - ncview **`JOBS/chem_phstatp/OUTPUT/chem_phstatp_3d.nc &`**
    - To look at vertical cross sections change "**`Axes`**" from **`Y Dim: y; X Dim: x`** to **`Y Dim: zu_3d; X Dim: x`**
    - Then move e.g. to y = 185 to reach a cross section in the middle of the simulation domain

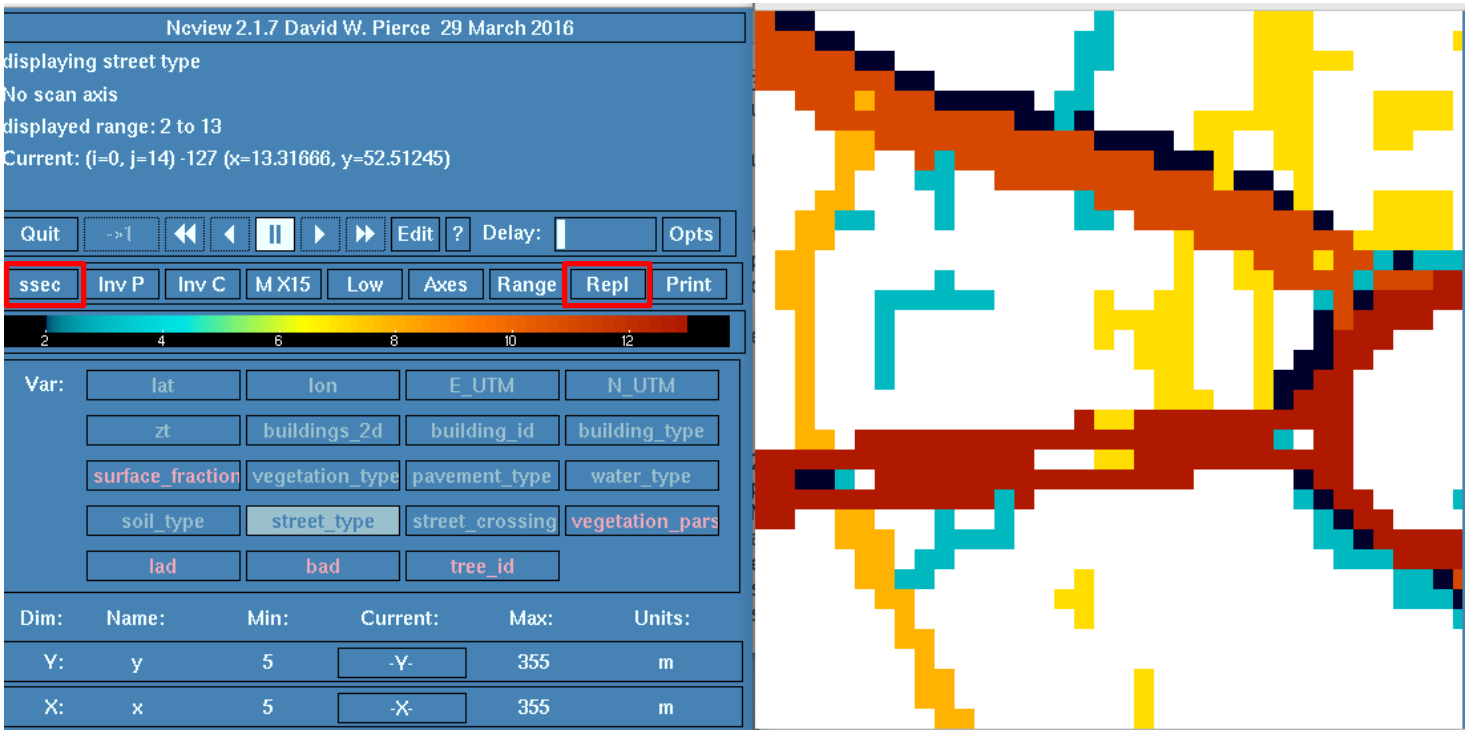
Which issues are possible when running PALM with the supplied setup?

- The size of the model domain is rather small, and the horizontal extent is less than the vertical extent.
- When the mixed layer grows after sunrise, larger eddies than the domain size will develop in reality. The development of eddies of this size is inhibited by the small model domain. This results in too weak turbulence, unstable instead of neutral stratification in the PBL and may affect the simulated PBL height.
- When the mixed layer grows further, it will hit the top of the model domain. Forget about the results already a bit before this happens!
- The chemistry needs some time before the simulation shows reasonable results! This time depends of the setup and its settings. Results right from the beginning of the simulation may not be realistic!
- This setup is just to be used to demonstrate the application of the chemistry model within a reasonable time. Please remember that the quality of the LES results will not be very good for this setup!

Results Preliminary question of Task 1

Where can I expect high traffic emissions in my domain?

The static file includes grid points with street type ≥ 11 (minimum index for main streets in the namelist). Parameterized emissions are highest on main streets.



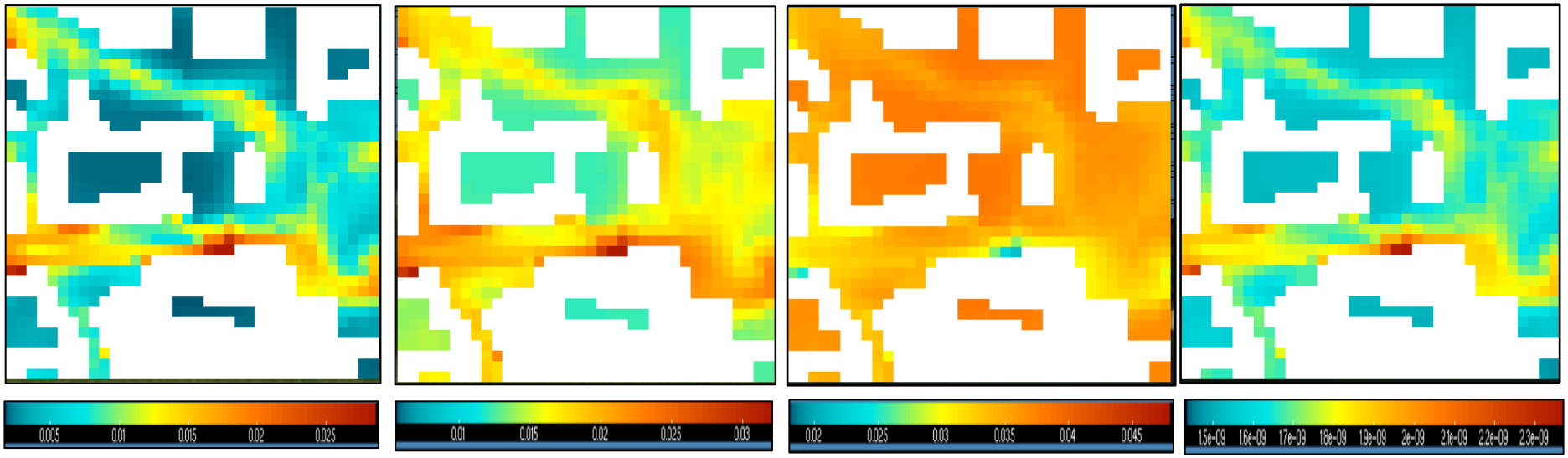
This figure and the following figures are created with the ncview option „Repl“ and color scheme „ssec“

Chemistry model exercise

Results Task 1

Concentrations at 7200 sec of instantaneous masked output for the lowest layer (5 m above ground) Figures from output of r22.04 (small differences to r23.04 due to differences in meteorology)

NO NO_2 O_3 PM10



Answers to question of Task 1

How do the concentrations of PM10, NO, NO_2 and ozone correlate?

Areas with local maxima of NO and NO_2 result in local minima for ozone (titration of ozone by NO).

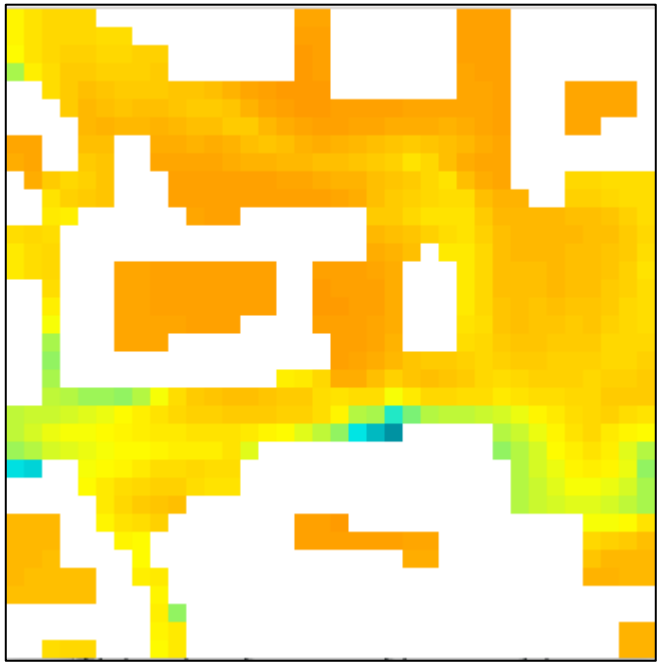
Chemistry model exercise

Results Task 2

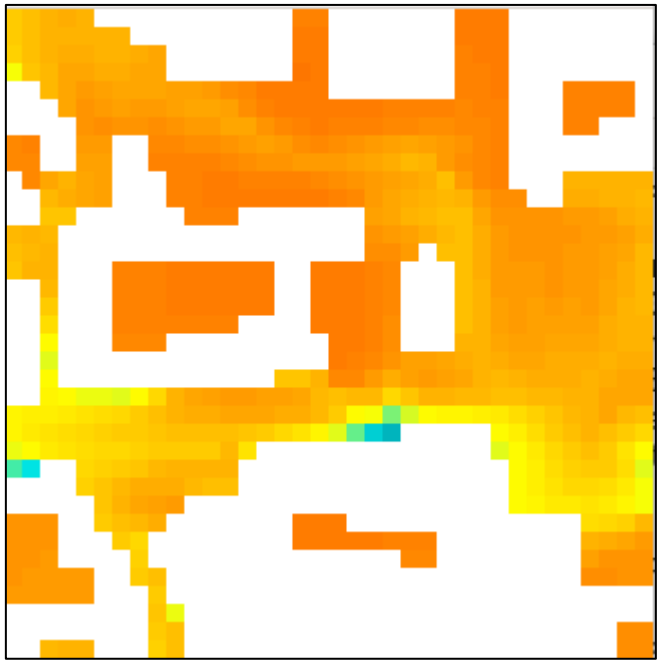
Analyzing results using ncview: Comparison of ‚phstatp' and ‚smog' results

Ozone at 7200 sec and 5 m height

phstatp



smog



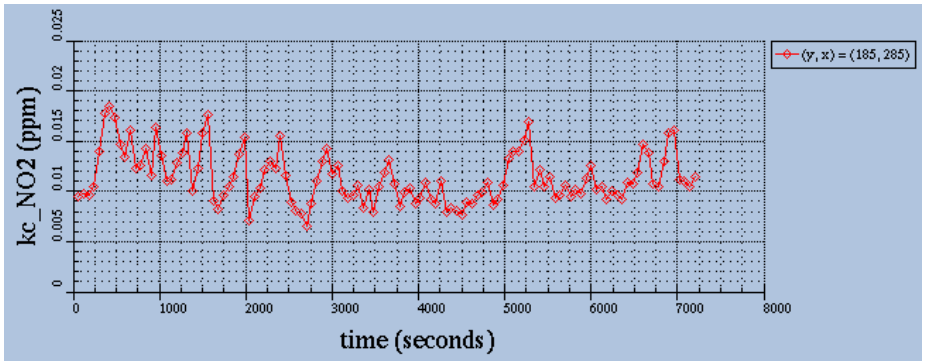
Chemistry model exercise

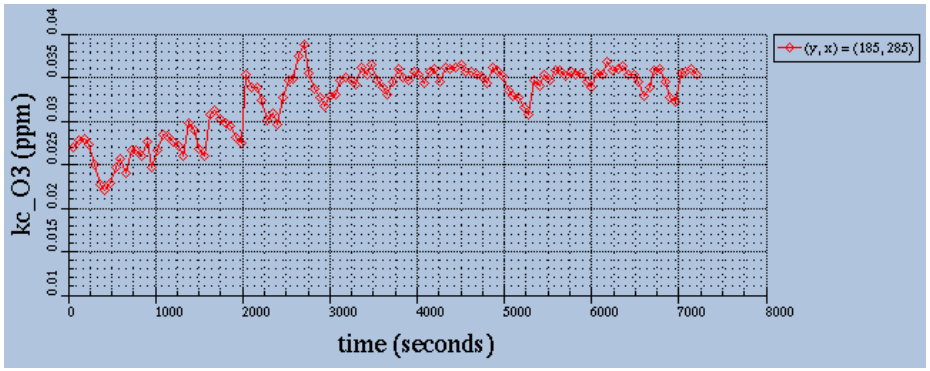
Results Task 2

Analyzing results using ncview: Comparison of ‚phstatp‘ and ‚smog‘ results

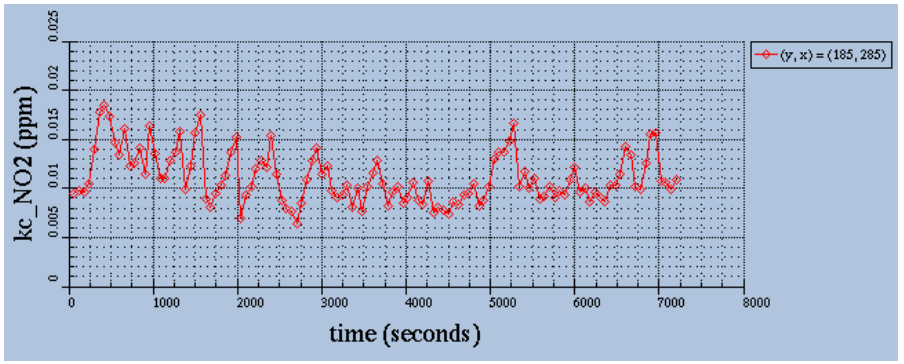
Time series at x=285m, y=185m for phstatp and smog

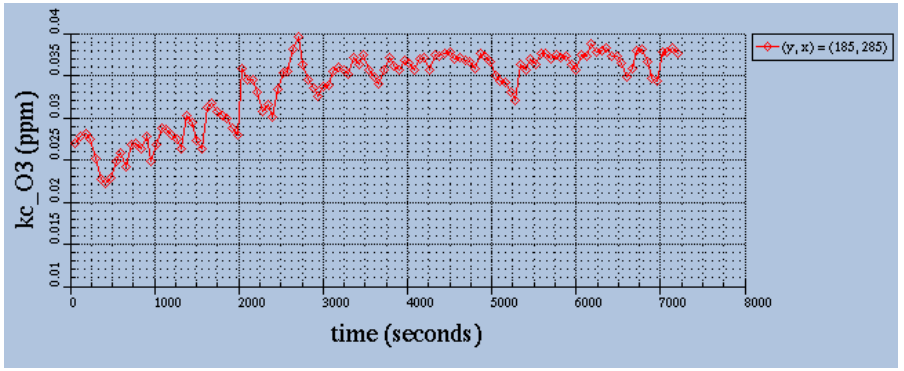
phstatp





smog





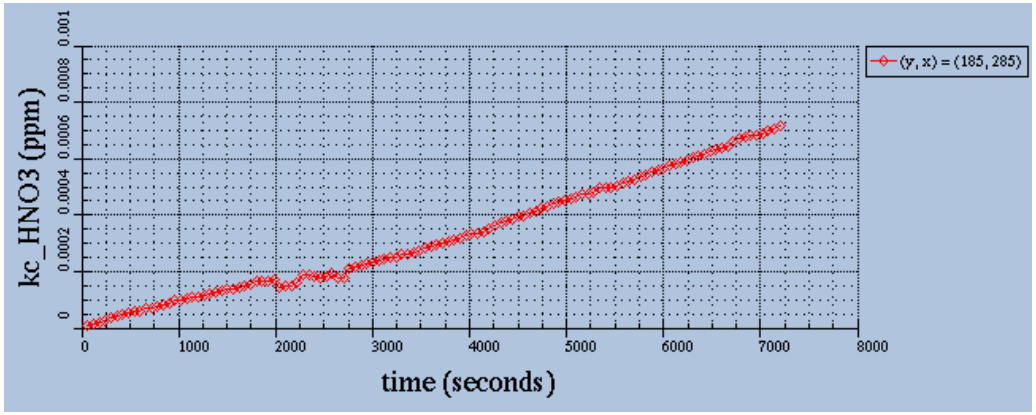
Chemistry model exercise

Results Task 2

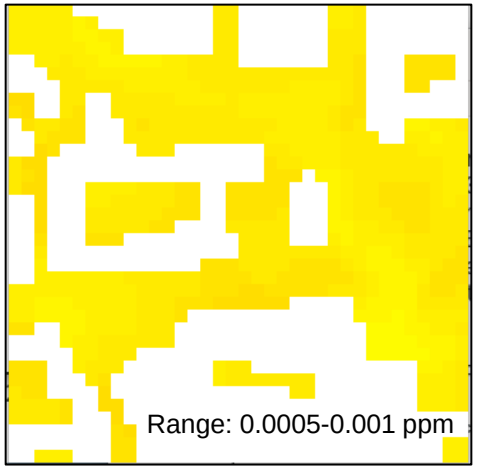
Analyzing results using ncview: Variables occuring only in ‚smog' mechanism

Products and radicals

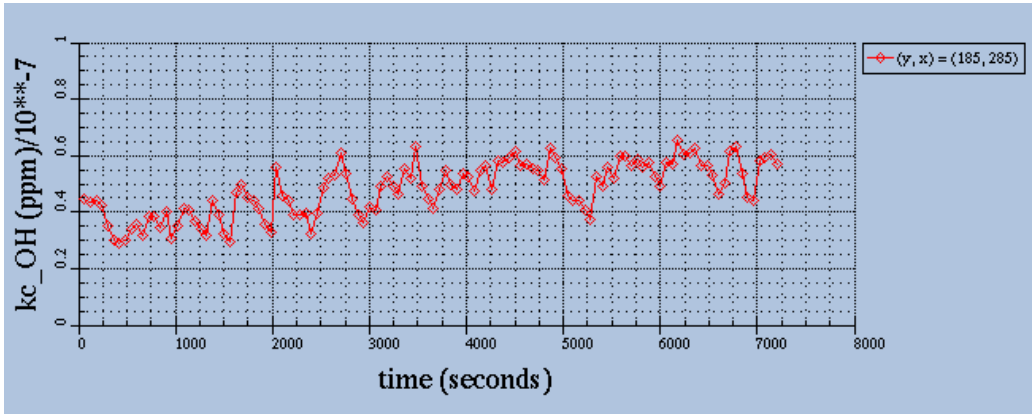
HNO_3



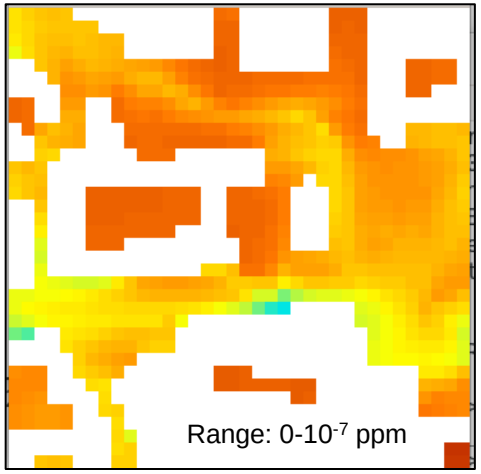
HNO_3 at 5m and 7200s



OH



OH at 5m and 7200s



Preliminary questions

(1) Where can we find the **`chem_gasphase_mod.f90`** for smog?

`packages/chemistry/kpp4palm/mechanisms/def_smog`

(2) What about PM10 when running PALM with smog?
Keep or remove? How can we find out?

PM10 does not occur in smog
(see **`chem_gasphase_mod.f90`** for smog, search for **`spc_names`**).

Another option is to look into
`packages/chemistry/kpp4palm/mechanisms/def_smog/smog.eqn`
Since PM10 does not occur in the smog mechanism, this variable is not known. The attempt to include PM10 in the output can result in a crash during runtime.

Question on simulation results

Why is ozone higher for smog than for phstatp?

Different from the photostationary equilibrium, where no net ozone production occurs, the smog mechanism includes a net production of ozone, HNO3 and PAN (RCOO2NO2).

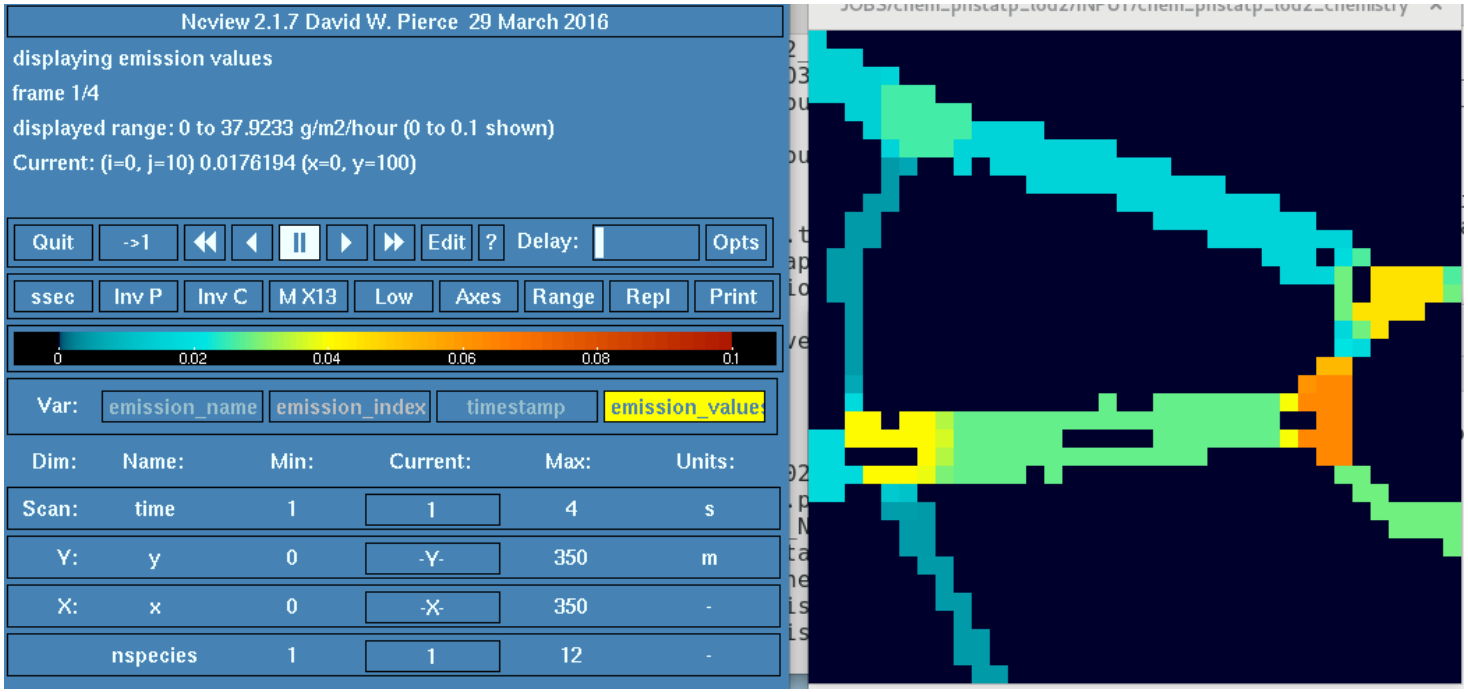
Due to the presence of aldehydes (RCHO) and hydrocarbons (RH) ozone is photochemically produced. After 7200 sec ozone near the ground is about 3 ppb higher for smog than for phstatp.

NO and NO_2 are marginally lower for smog than for phstatp since NO_x is consumed when HNO_3 and PAN are produced.
The small differences in ozone, NO_2 and NO indicate that the use of photostationary equilibrium mechanism is sufficient to simulate these compounds under urban conditions for short simulations. This is especially the case in our setup because the simulation ends at 9 h local time.

Preliminary question

Find order of compounds in files with **`ncdump -v emission_name JOBS/chem_phstatp_lod2/INPUT/chem_phstatp_lod2_chemistry`**

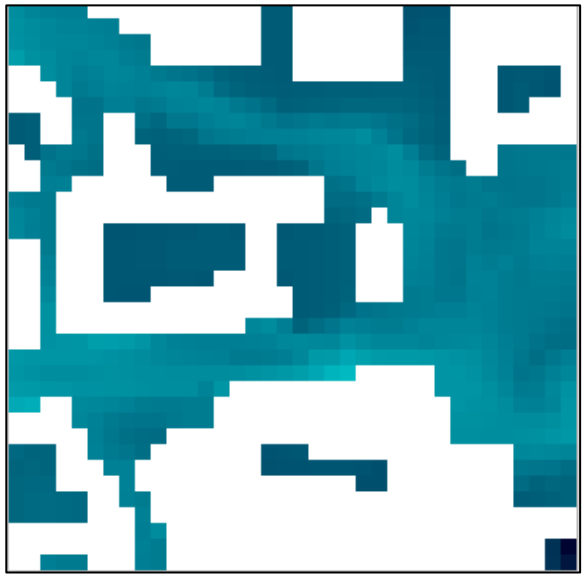
NO emission (first emission_value)



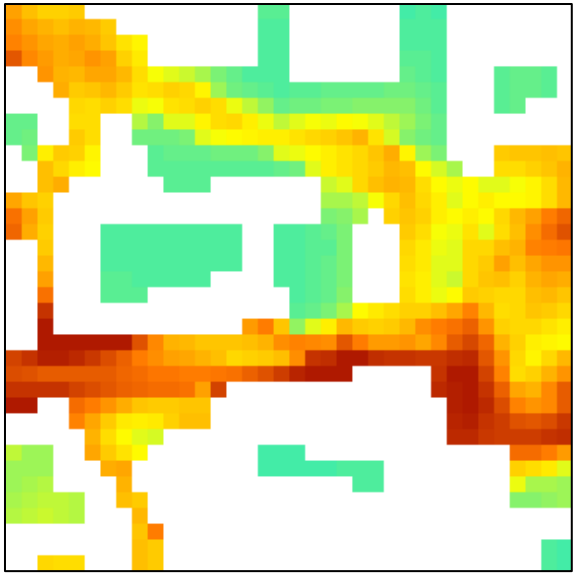
Analyzing results using ncview: Comparison of LOD0 and LOD2 runs

- PM10 in kg m^{-3} at 7200 sec. at surface

LOD 0



LOD 2

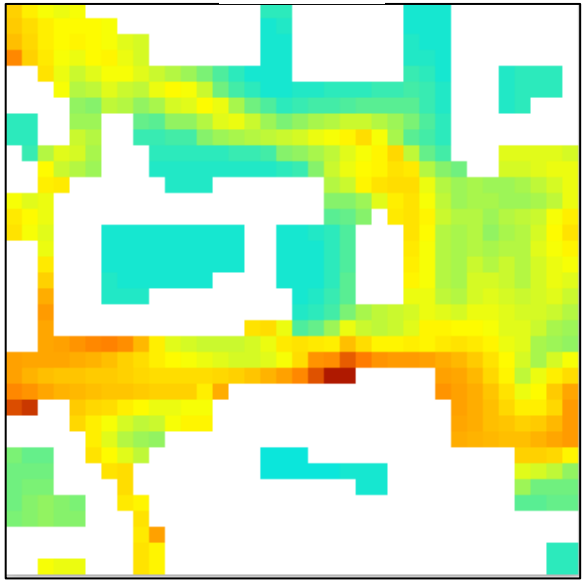


Results Task 3

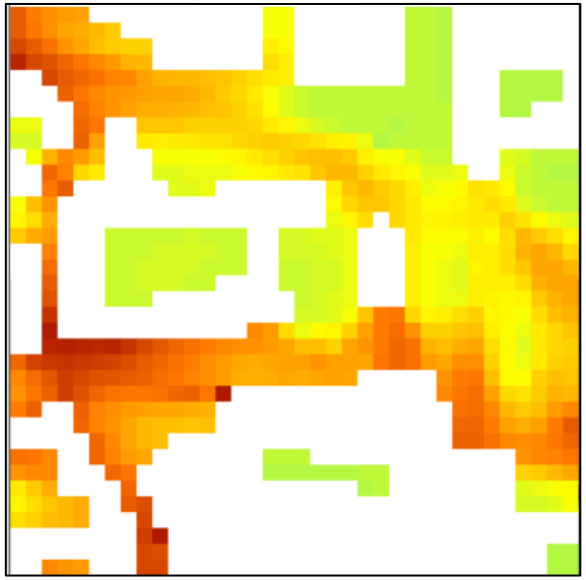
Analyzing results using ncview: Comparison of LOD0 and LOD2 runs

- NO_2 in ppm at 7200 sec. at surface

LOD 0



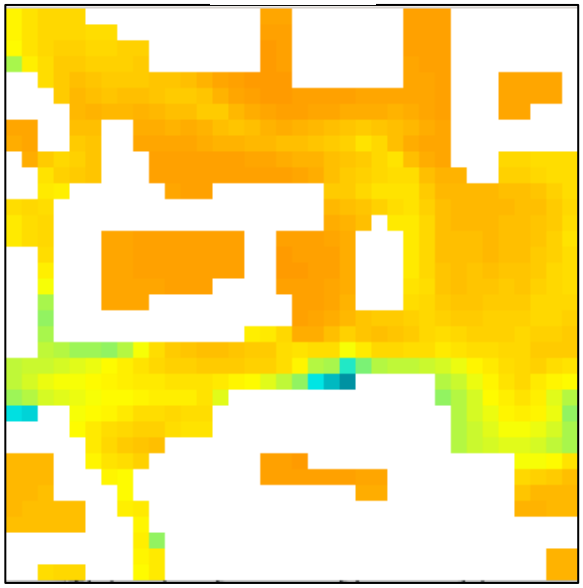
LOD 2



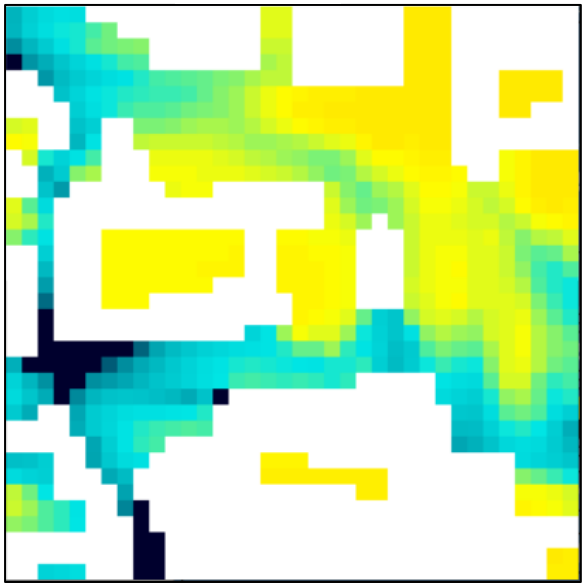
Analyzing results using ncview: Comparison of LOD0 and LOD2 runs

- O_3 in ppm at 7200 sec. at surface

LOD 0



LOD 2



Preliminary question

Take a look at the emission fields within the chemistry driver `chem_phstatp_lod2` using ncview. What is eye-catching when looking into the data?

Traffic emissions differ for the different main streets and also along a street. Emissions are especially enhanced at junctions. This is due to the fact that car emissions are increased by stop and go and acceleration processes. Furthermore one can see that emissions on side roads are significantly lower than on main roads.

The approach for parameterized emissions (LOD 0) only allows for uniform emissions on and along all main roads and side roads, respectively. Furthermore, other than for the LOD 2 emission data set there is no temperature dependency in the emission data. Also, for PM, only exhaust emissions are considered when using LOD 0 while the applied LOD 2 emission data set includes an approach, which considers PM emissions via particle resuspension.

Question on simulation results

How much do the results using LOD 2 emission input differ from those of Task 1? Can you explain the differences based on the description of the different emission inputs?

For PM10, surface concentrations are significantly higher when using the LOD2 emission data set (approx. 15 µg m^{-3}) compared by using the LOD 0 emission option (approx. 2 µg m^{-3}). This difference is mainly due to the fact that LOD 0 only considers PM exhaust emissions and no particle resuspension processes. Furthermore, no stop and go and acceleration processes are considered leading also to comparatively lower emissions. The latter also holds for NO and NO_2 emissions, which are also higher than for LOD 0.

Looking at O_3 which is a secondary pollutant we can see the impact on the chemistry using the different emission options. As O_3 is destroyed by NO, its concentrations are higher for the LOD 0 run than for the LOD 2 run with higher NO concentrations.