Model performance evaluation and computational efficiency of chemical mechanisms implemented in the microscale urban climate model PALM-4U

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MOSAIK

Introduction

In the purview of the joint project **MOSAIK** (https://palm.muk.uni-hannover.de/ mosaic), a new state-of-the-art microscale urban climate model (PALM-4U) is developed to accurately simulate city to local scale urban canopy processes such as urban heat island, ventilation in street canyons, and air pollution hotspots etc at turbulence resolving scales. PALM-4U is based on the well established LES model PALM (Maronga et al., 2015). PALM-4U includes a chemistry module to describe transport, chemical transformation and removal of pollutants. This work evaluates computational efficiency of the chemistry model and performance of the 4 chemical mechanisms implemented in PALM-4U.

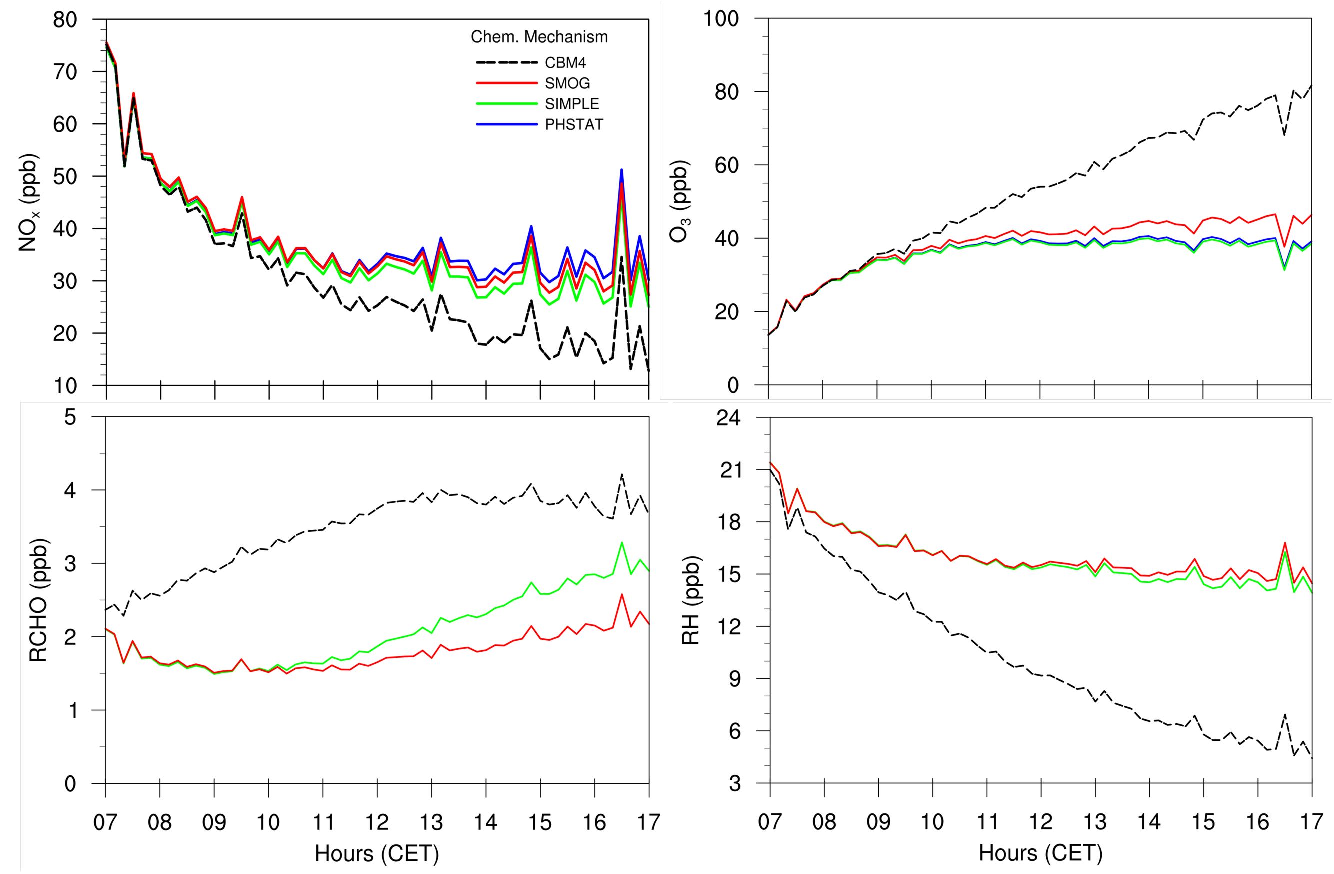
Chemistry Module in PALM-4U

- Fully coupled 'online' chemistry;
- Automatic generation of the chemistry code with the **K**inetic **P**re-**P**rocessor (KPP, Damian et al., 2002);
- Adapted version of the KP4 post-processor (Jöckel et al., 2010) for the choice of gas phase chemical mechanisms;
- A simple photolysis parameterization;
- Emission module
- Deposition module
- An aerosol module (SALSA, Kokkola et al, 2008).
- Currently PALM-4U includes the following chemistry mechanisms:
  - ***CBM4:*** *Carbon Bond Mechanism (Gery et al. 1989, 32 compounds, 81 reactions)*
  - ***SMOG:*** *Photochemical smog mechanism (13 compounds, 12 reactions)*
  - ***SIMPLE:*** *Simplified of SMOG (9 compounds, 7 reactions)*
  - ***PHSTAT:*** *Photo-stationary state (3 compounds, 2 reactions)*
  - ***PASSIVE:*** Only 2 passive tracers, no chemical reactions.

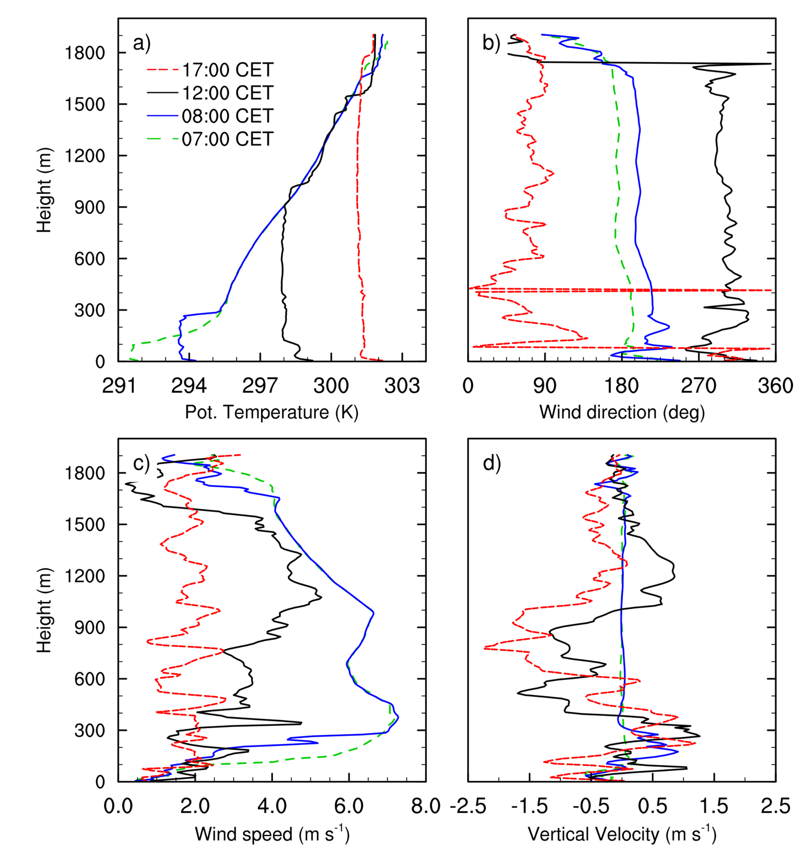
Comparison of 4 Chemical Mechanisms Over an Urban Quarter of Berlin (Germany)

Four chemical mechanism described above have been evaluated. Being the most detailed and largely validated, the CBM4 mechanism has been used as a reference. Following is the simulation setup :

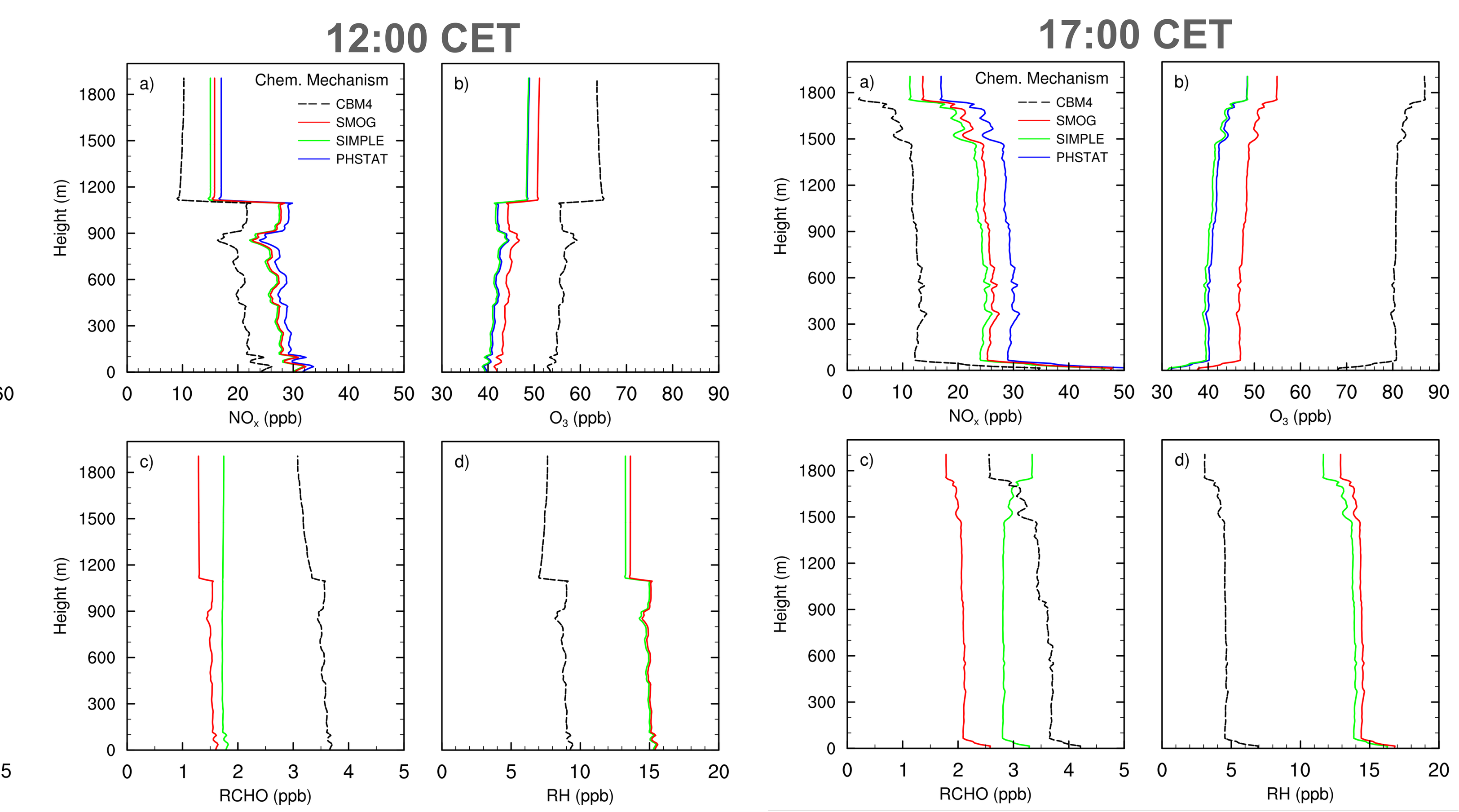
- Domain: Ernst-Reuter-Platz, Berlin, a large round-about with some high-rise buildings and heavy car traffic.
- Start: 21 July, 00:00 UTC; Simulation length = 17 hours
- nx = ny = 96, nz = 192; dx=dy=dz =10 m; Lateral Boundaries: INIFOR (from COSMO regional scale model)
- Traffic emissions depending on the street type from OpenStreetMap:
  Emission Factors: main streets = 1.667; side streets = 0.334



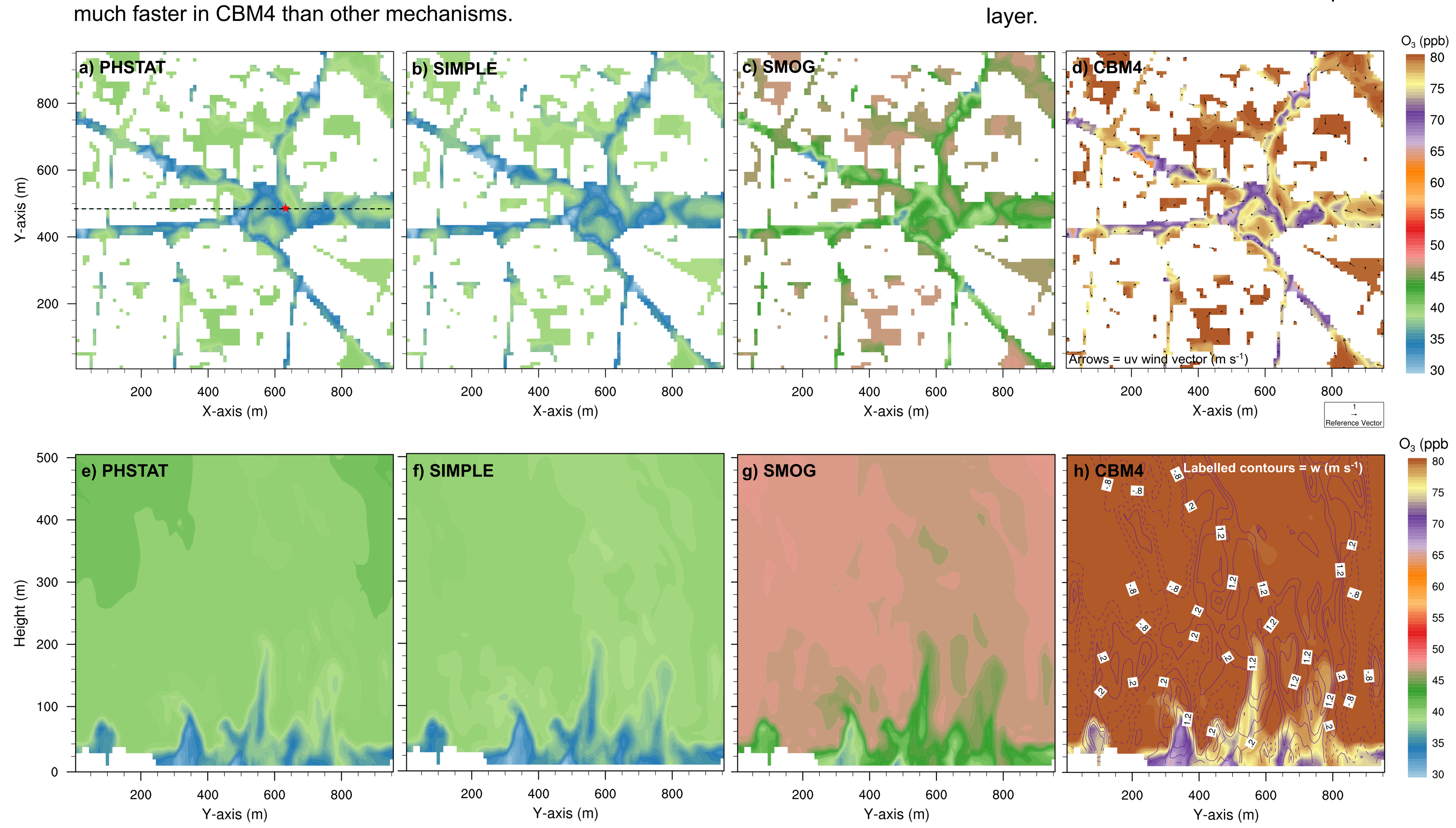
Time series plots of chemical species concentrations simulated with 4 different chemical mechanisms. The location is indicated by star in figure 'a' below. NO_x and RH are spent much faster in CBM4 than other mechanisms.



Profiles of meteorological quantities indicating evolution and structure of the atmospheric boundary layer.

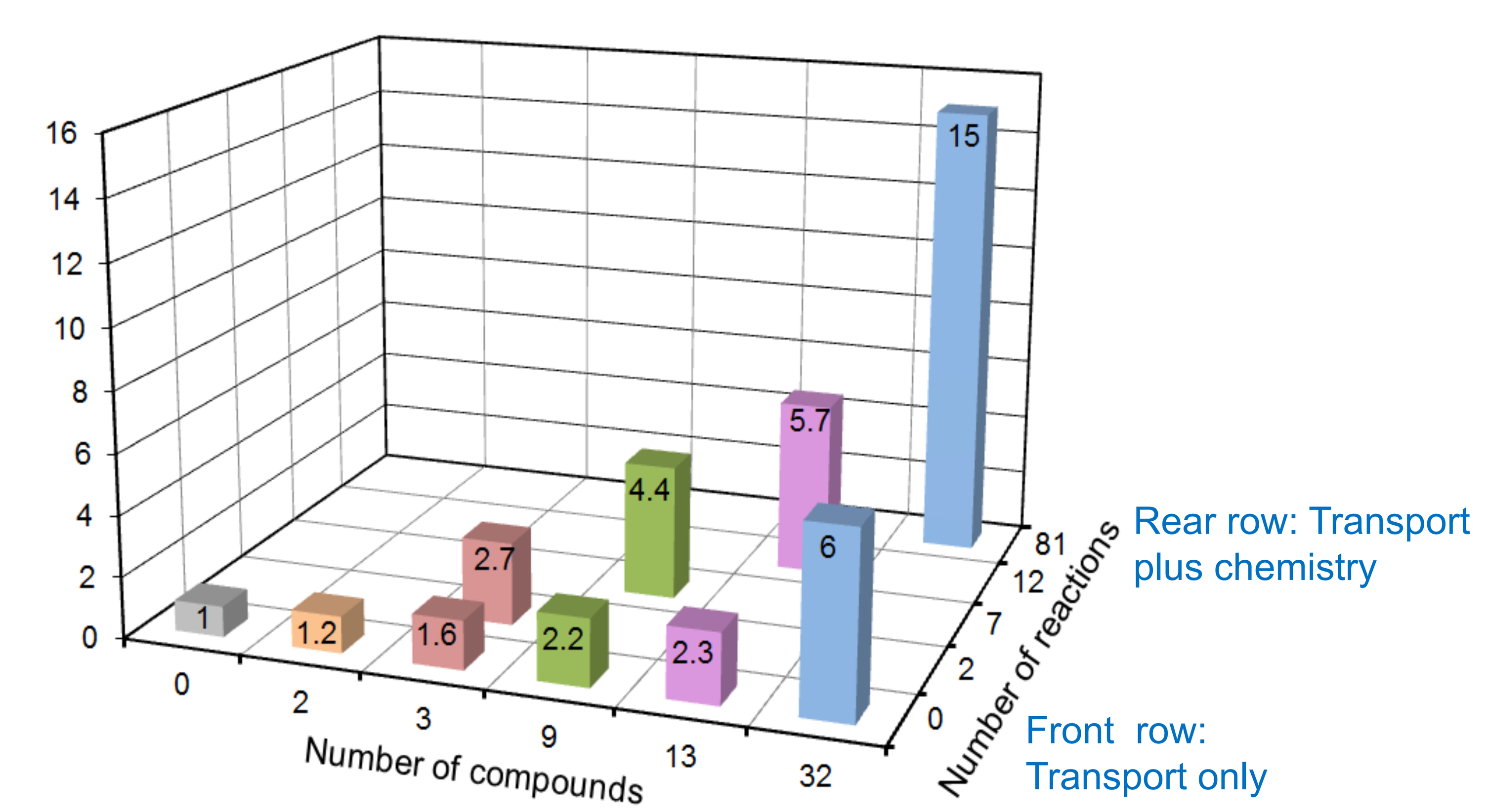


Vertical profiles of chemical species at 1200 CET and 1700 CET on 21 July 2013. Compared to other mechanisms, CBM4 simulated highest O_3 and RCHO and lowest NO_X and RH during day time.



Horizontal and vertical cross-sections of O_3 concentration at 1700 CET, at Ersnst-Reuter-Platz, Berlin, Germany, indicating differences in concentration patterns and magnitude of O_3 amongst four chemical mechanism. Black dashed line in figure 'a' indicates location of the vertical cross-section and star indicates location of time series and profile data.

Computational Demand of Chemistry



CPU time requirement of PASSIVE (orange), PHSTAT (red), SIMPLE (green), SMOG (purple) and CBM4 (blue) relative to a meteorology only run (gray).

Conclusion and Outlook

Spatial distribution (horizontal and vertical) of chemical species show turbulence resolved transport of atmospheric pollutants. Difference in O_3 between CBM4 and other mechanisms are quite large. Since most of the chemical mechanisms are primarily designed for regional and global scale models, therefore, these mechanisms are almost unaffordable for computationally expensive LES models. It is important to design highly condensed chemical mechanisms for turbulence resolved microscale simulations. However, applying highly simplified mechanisms can also be a source of increased uncertainty in the chemistry output. PALM-4U is still under extensive development, further chemistry mechanisms are being evaluated to be added to PALM-4U, while already implemented mechanisms are undergoing extensive testing. Work is in progress to include new features such as lateral boundary conditions for chemical species, photolysis schemes, aerosols schemes etc. Accounting for shading effects within the photolysis parameterization is intended.

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