Institute for Meteorology and Climate Research

Atmospheric Environmental Research (IMK-IFU)

Implementation of an Online Chemistry Model to a Large Eddy Simulation Model

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Introduction

Accurate representation of dispersion, chemical transformation and removal of air pollutants requires fine-scale turbulence-resolving simulations that could explicitly resolve building structures, surface heat fluxes at building facades, street canyons and terrain variations. Large Eddy Simulation (LES) models permit to resolve relevant scales of turbulent motion, so that these models can capture the inherent unsteadiness of atmospheric turbulence. However, so far, LES models are hardly applied for urban air quality studies.

In this context, a new urban climate model (UCM) is developed within the joint project **MOSAIK** (**Mo**dellbasierte **S**tadtplanung und **A**nwendung **i**m **K**limawandel: Model-based city planning and application in climate change) under the lead of the Institute of Meteorology and Climatology at the Leibniz Universität Hannover. The new urban climate model PALM-4U is based on the state-of-the-art **Pa**rallelized **L**arge-Eddy Simulation **M**odel (PALM, Maronga et al, 2015).
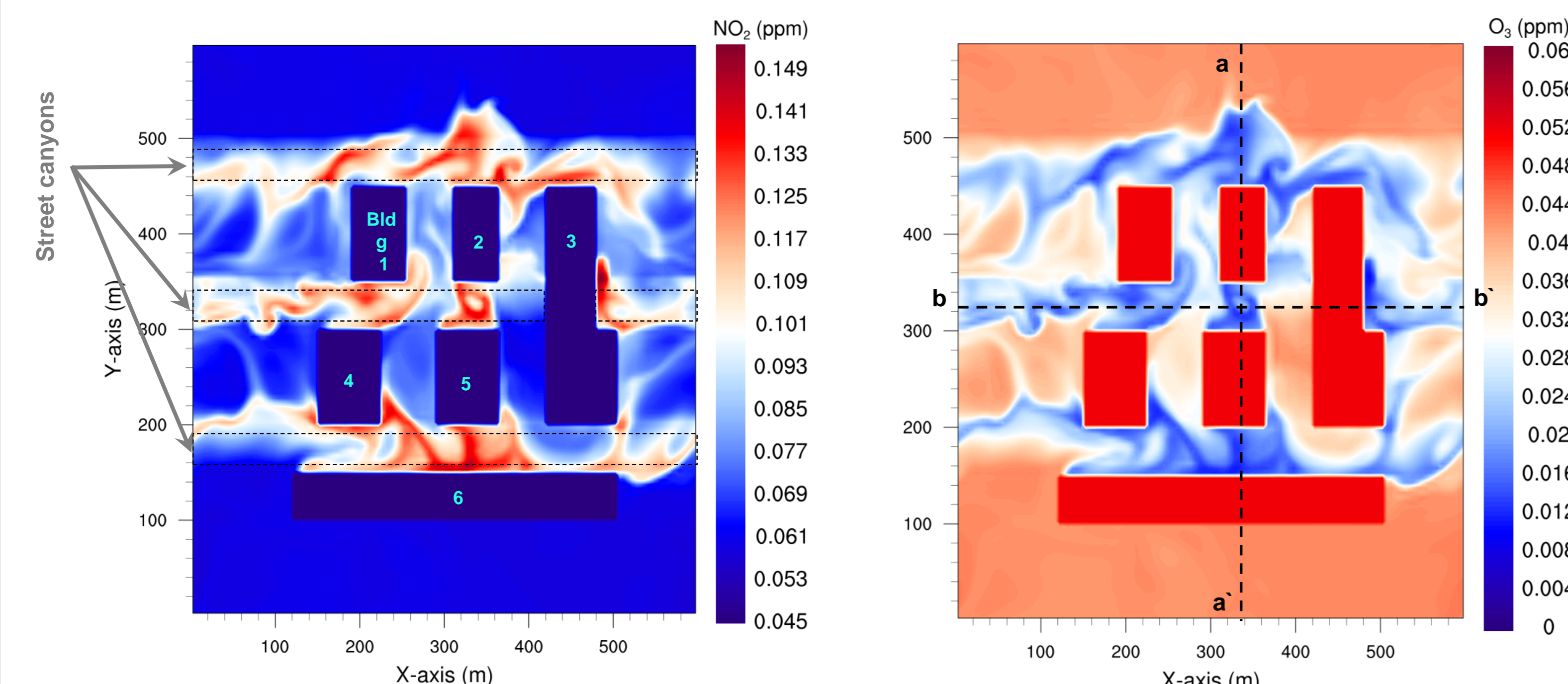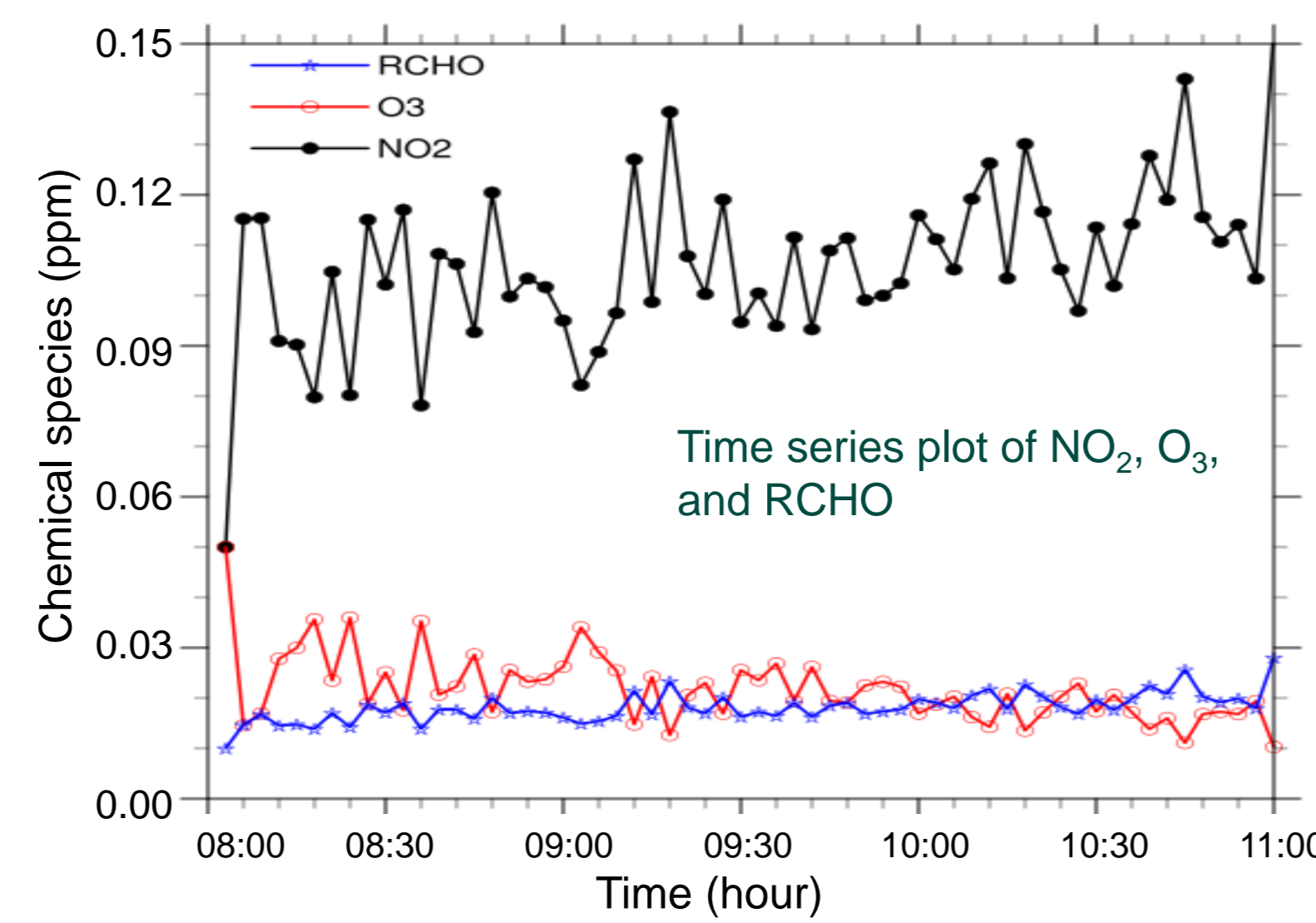
A fully coupled 'online' chemistry model has been developed and implemented into PALM. Kinetic PreProcessor (KPP), has been utilized for the numerical integration of gas phase chemical reactions. Reduced chemical mechanisms with only a small number of products have been implemented including CO and a O_3-NO_2-NO-VOC-HO_x chemistry.

Model Setup

Domain size : nx = ny = 120, nz = 120 ;
dx = dy = dz = 5 m
Latitude = 50° ; Day and time = 6 July, 08:00 LT;
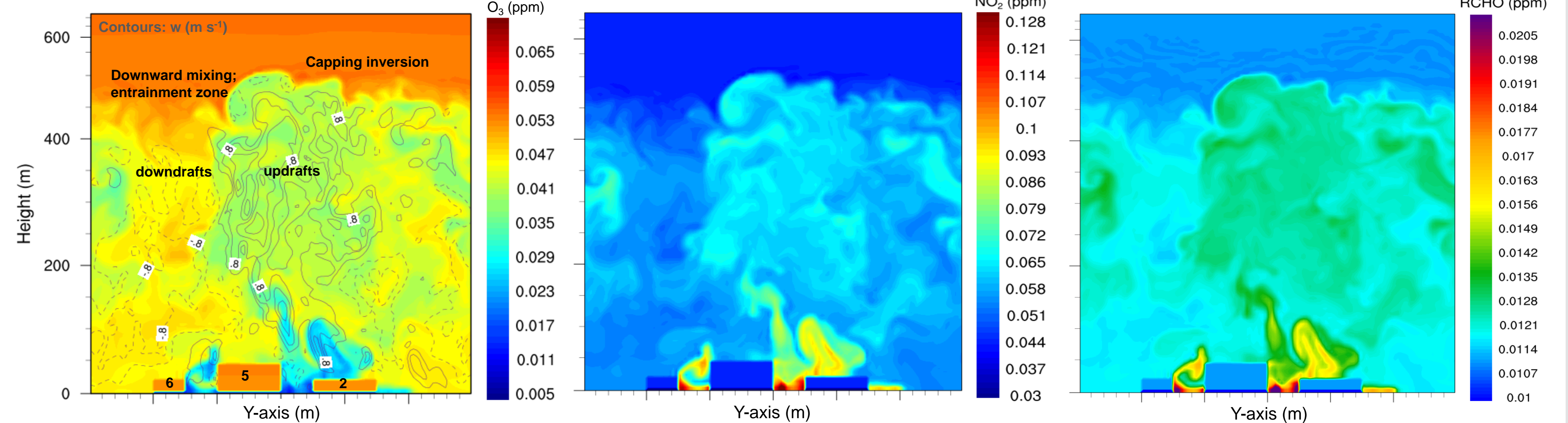U = 1.0 m s^{-1}; Surface heat flux = 0.06 K m s^{-1};

Chemistry:
Photolysis: Simple parameterization
Initial Values (ppm): NO = 0.01; NO_2 = 0.05;
O_3 = 0.05; RH = 0.001; RCHO = 0.01.
Emission rates (µg m^{-2} s^{-1}): RH = 0.001;
NO_2= 0.002; NO = 0.01

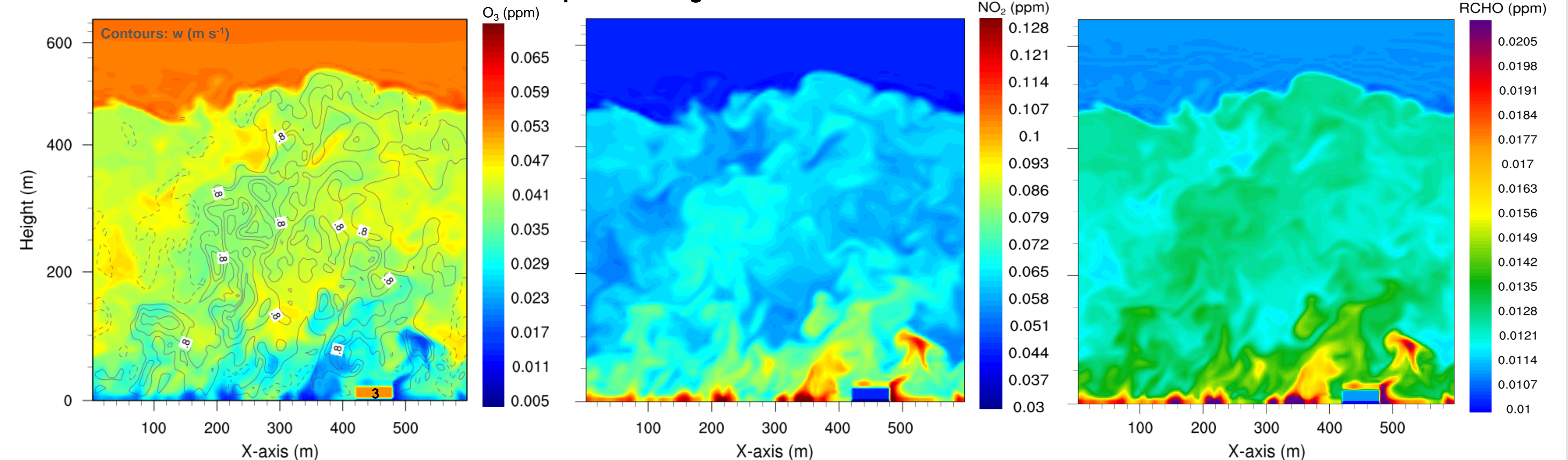**Topographic Setup:** Three street canyons in W-E direction with 6 building blocks of varying heights.

Time series plot of NO_2, O_3, and RCHO

Chemical transformation and transport of NO_2 and O_3 near the surface. NO_2, NO, OH and RH are emitted from street canyons (indicated as dashed boxes in the left panel) at a constant rate. Black dashed lines in the right panel show locations of Y-Z and X-Z vertical cross sections.

Y-Z Vertical cross sections for 3 chemical species along transect aa`

X-Z vertical cross sections for 3 chemical species along transect bb`

Chemical Mechanism

$NO_2 + hv \rightarrow NO + O_3$
$O_3 + hv \rightarrow 2OH + O_2$
$NO + O_3 \rightarrow NO_2$
$RH + OH \rightarrow RO_2 + H_2O$
$RO_2 + NO \rightarrow NO_2 + RCHO + HO_2$
$HO_2 + NO \rightarrow NO_2 + OH$

Conclusion and Outlook:

The chemistry model for PALM-4U is able to successfully simulate chemical transformation and transport of the chemical species. Results show a strong effect of turbulent structures on simulated pollutant concentration fields.
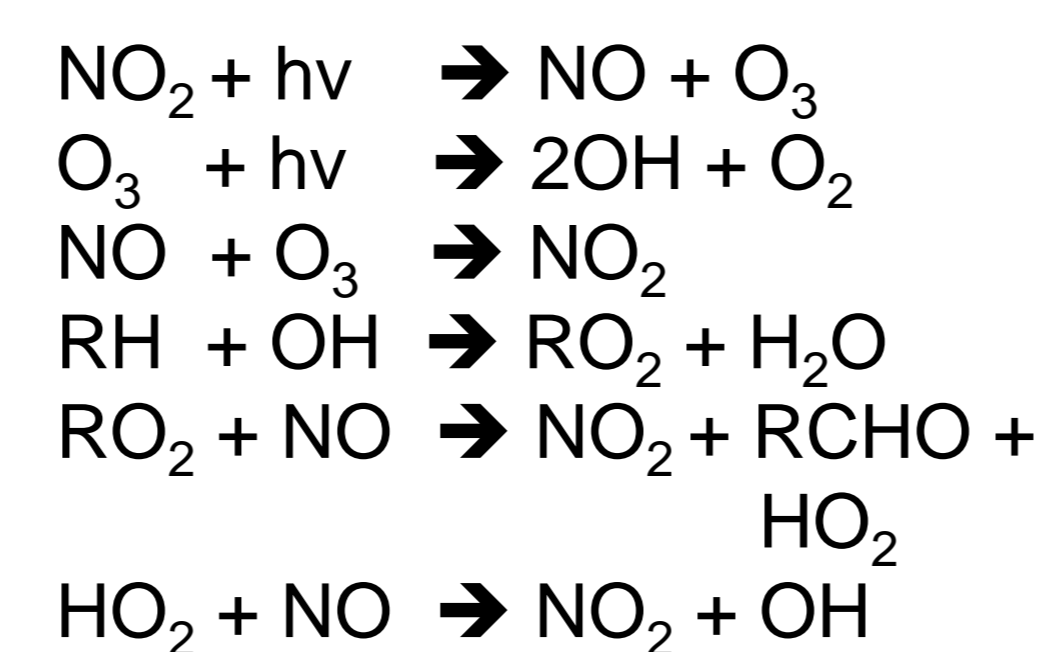
The following features are planned to be introduced in the future:
a) External forcing from regional scale models; b) nesting, c) emission and deposition process; c) Aerosol chemistry, and, d) RANS (Reynolds-Averaged-Navier-Stokes mode.

References:

Maronga et al, 2015, Geosci. Model Dev. 8, doi:10.5194/gmd-8-2515-2015;
MOSAIK web page: https://palm.muk.uni-hannover.de/mosaik/wiki
PALM web page and reference: https://palm.muk.uni-hannover.de/trac
KPP web page: http://people.cs.vt.edu/asandu/Software/Kpp/

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