# Development and Implementation of an Online Chemistry Module to a Large Eddy Simulation Model for the Application in the Urban Canopy

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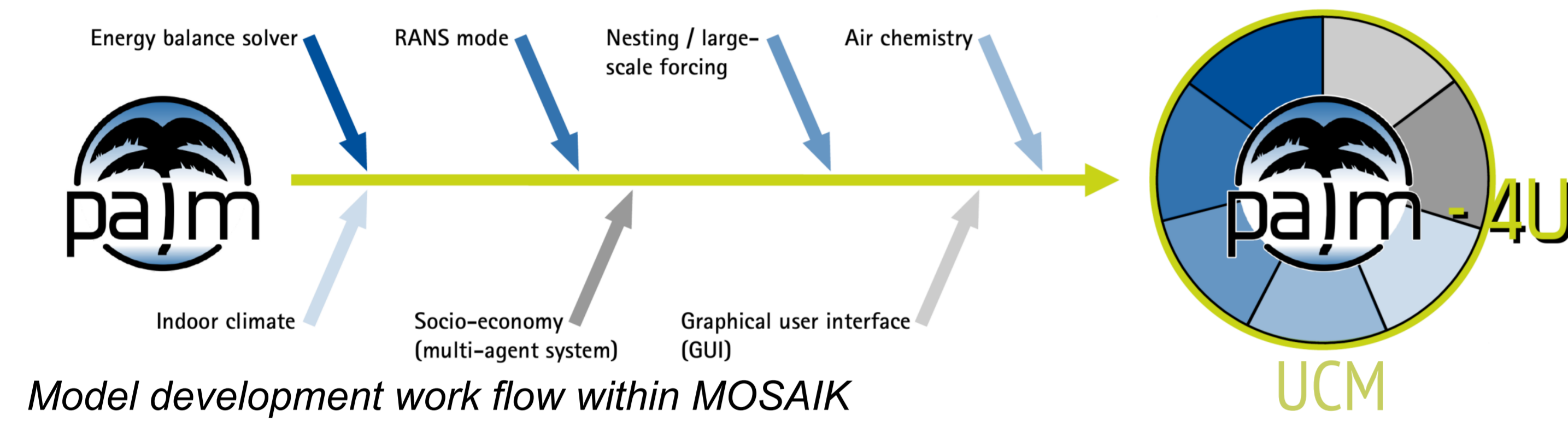
## Introduction

Adequate modelling tools are required to support urban planning and the development of strategies aiming at minimizing adverse effects on urban climate such as poor air quality. However, a realistic implementation of urban canopy processes still poses a serious challenge for current weather and air quality models due to the small scale of the phenomena to be described.

To address this demand, a new micro-scale 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 model PALM-4U is based on the state-of-the-art large-eddy simulation (LES) model PALM (Maronga et al., 2015). The final operational version of PALM-4U will be distributed as Open Source software and will include modules for atmospheric chemistry, indoor climate and energy demand and human-related quantities (physiological equivalent temperature or universal thermal climate index). Furthermore, it will be coupled to a multi-agent model.

Due to the high computational demands of an LES based model a RANS mode is also being developed.


Model development work flow within MOSAIK



Time series of $O_3$, RH, NO, $NO_2$ (left) and vertical profiles of $NO_2$, $O_3$ at different times (right) at location ★
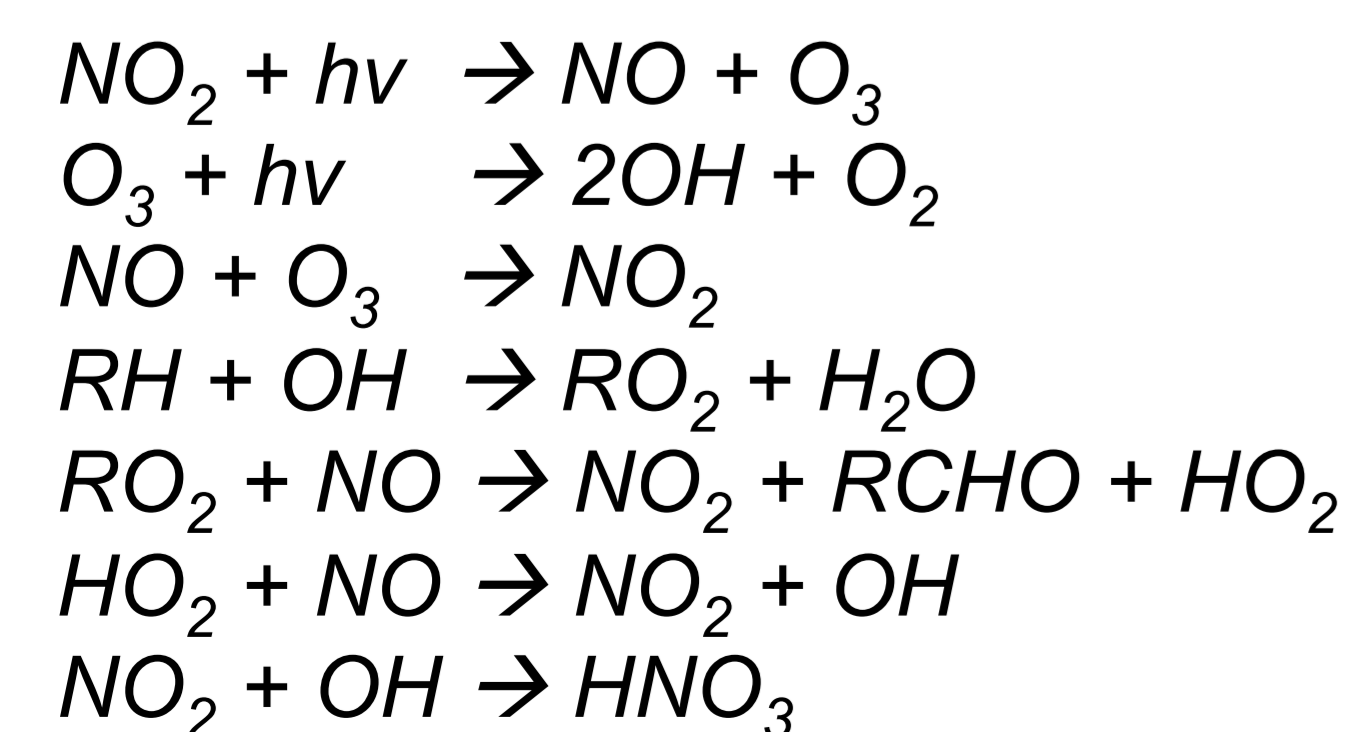
## Implementation of the Chemistry Module in PALM-4U

A fully coupled 'online' chemistry model has been implemented into PALM-4U. Automatic generation of the chemistry code with the **K**inetic **P**re-**P**rocessor (KPP, Damian et al., 2002) allows for high flexibility in the choice of gas phase chemical mechanisms of different complexity. Currently PALM-4U includes the following chemistry options:

- *CBM4* (Carbon Bond Mechanism, Gery et al. 1989, 32 compounds, 81 reactions)
- *SMOG* (a simple photochemical smog mechanism, 13 compounds, 12 reactions)
- *SIMPLE* (further simplification of SMOG, 9 compounds, 7 reactions)
- *PHSTAT* (photo-stationary state only, 3 compounds, 2 reactions)
- *PASSIVE* (just 2 passive tracers, no chemical reactions)

A simple photolysis parameterization is implemented in PALM-4U. A two-way LES-LES nesting is also implemented in PALM-4U which makes it possible to zoom in smaller areas for high resolution simulation.



Concentration of $NO_2$ (top) and $O_3$ (bottom) at 13:30 UTC

Z-Y-vertical cross section at line aa': Concentration (shaded color) of $NO_2$ (top) and $O_3$ (bottom) and W (-2.0 to 2.0 m s$^{-1}$, negative values as dashed lines) at 5:30 UTC (left) and 13:30 UTC (right)

## Case Study for an Urban Quarter of Berlin (Germany)

*SIMPLE* mechanism:

$$NO_2 + hv \rightarrow NO + O_3$$
$$O_3 + hv \rightarrow 2OH + O_2$$
$$NO + O_3 \rightarrow NO_2$$
$$RH + OH \rightarrow RO_2 + H_2O$$
$$RO_2 + NO \rightarrow NO_2 + RCHO + HO_2$$
$$HO_2 + NO \rightarrow NO_2 + OH$$
$$NO_2 + OH \rightarrow HNO_3$$

➢ Domain: Small area of Berlin around Ernst-Reuter-Platz, a large roundabout with some high buildings and heavy car traffic
➢ Start: 21 July, 5:00 UTC; Simulation length = 9 hours
➢ nx = ny = 96, nz = 120; dx=dy=dz =10 m; ug = vg = 1.0 m s$^{-1}$
➢ Modules: urban surface model, land surface model, canopy model, radiation, photolysis model, chemistry model
➢ Traffic emissions parameterized depending on the street type classes from OpenStreetMap: NO= 39.550 ug m$^{-2}$ s$^{-1}$; $NO_2$= 16.950 ug m$^{-2}$ s$^{-1}$; RH= 12.625 ug m$^{-2}$ s$^{-1}$
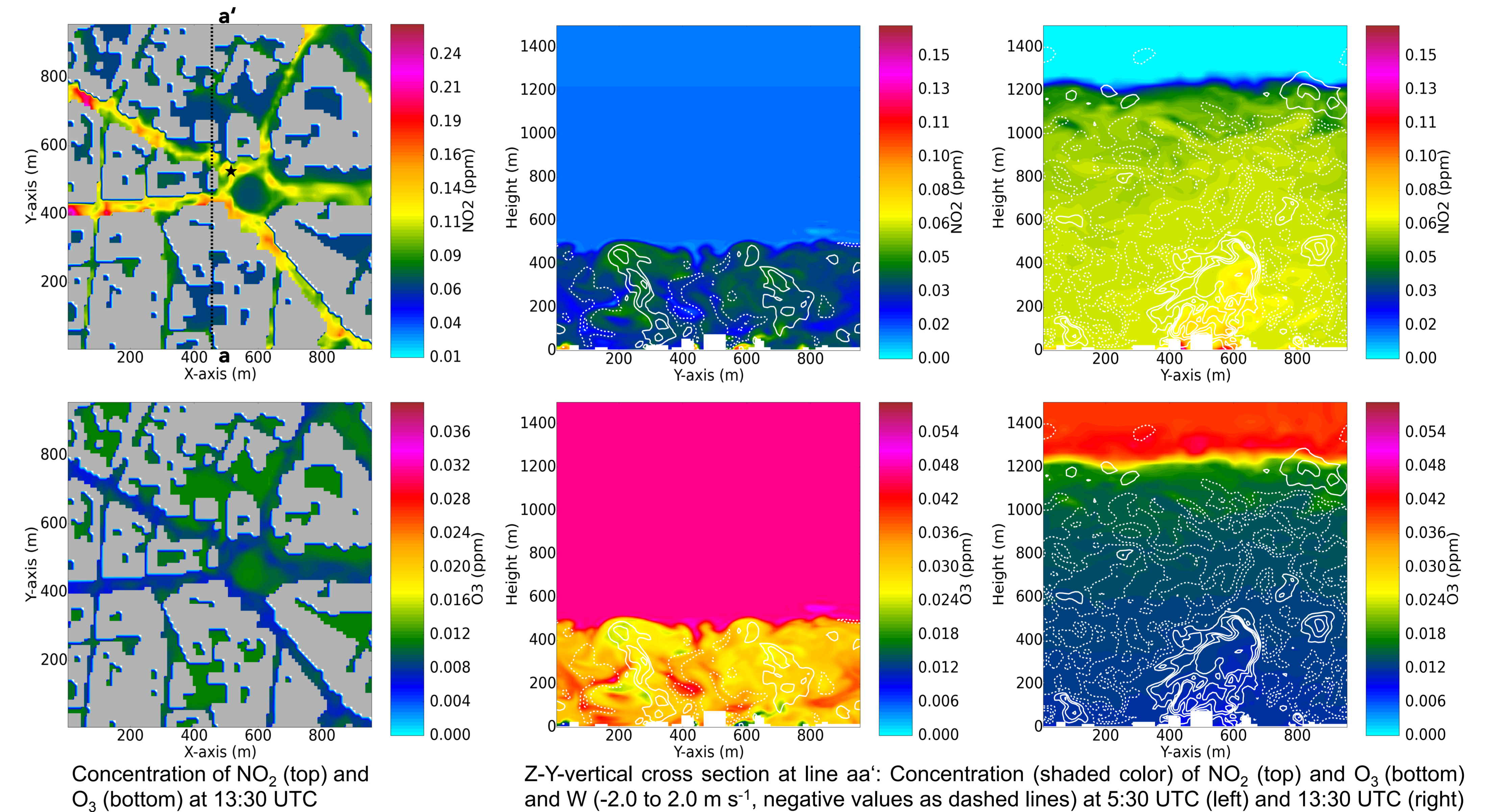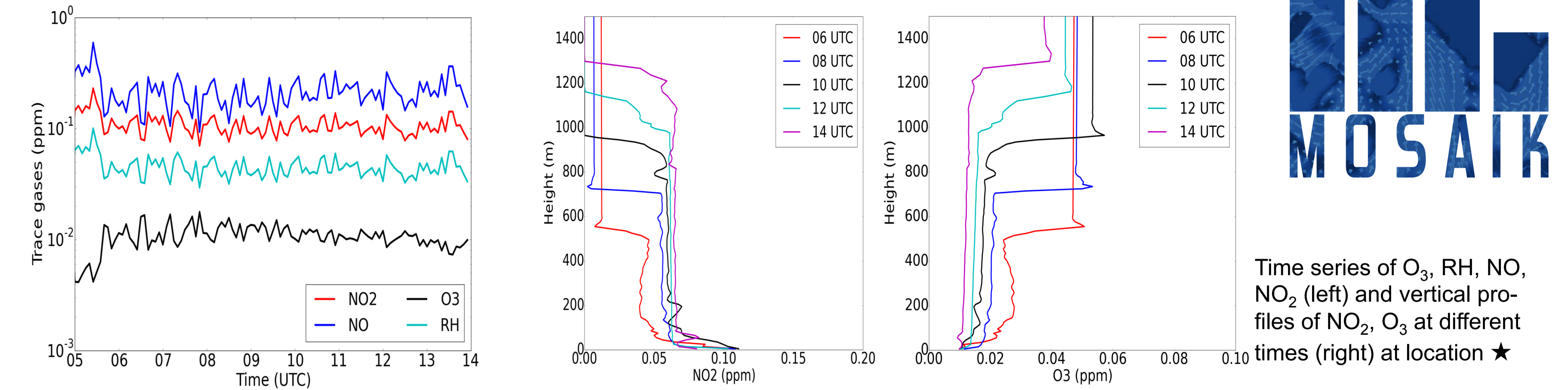
## Outlook

PALM-4U is still under extensive development, which also holds for its chemistry module. Different mechanisms will be added and already implemented mechanisms undergo further testing. Efforts will be made to speed up chemistry (vector version, larger time steps for chemistry). Accounting for shading effects within the photolysis parameterization is intended. The implementation of an aerosol module (SALSA, Kokkola et al, 2008), which is coupled to the gas phase chemistry is currently tested and the introduction of deposition processes is planned.

**References:**

MOSAIK web page: https://palm.muk.uni-hannover.de/mosaik/wiki
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