



GEFÖRDERT VOM



Bundesministerium  
für Bildung  
und Forschung



# Development and Application of an Online Coupled Chemistry Urban Microscale Model PALM-4U

**Basit Khan<sup>1</sup>, Renate Forkel<sup>1</sup>, Sabine Banzhaf<sup>2</sup>, Emmanuele Russo<sup>2</sup>, Farah Kanani-Sühring<sup>3</sup>, Matthias Mauder<sup>1</sup>, Björn Maronga<sup>3</sup>, Siegfried Raasch<sup>3</sup>, Mona Kurppa<sup>4</sup>, and Klaus Ketelsen<sup>5</sup>**

*<sup>1</sup>Karlsruher Institut für Technologie (IMK-IFU), <sup>2</sup>Freie Universität Berlin (FUB), Institute of Meteorology, TrUmf, <sup>3</sup>Leibniz Universität Hannover (LUH), IMUK, <sup>4</sup>University of Helsinki, <sup>5</sup>Independent Software Consultant*

# OUTLINE

## □ Background

- The MOSAIK Project
- PALM, The LES Model
- PALM-4U - Components

## □ Chemistry in PALM-4U

- Interface between Chemistry and PALM-4U
- Current Features

## □ A Case Study from Downtown Berlin-Germany

- Model Setup
- Simulation Domain
- Results

## □ Summary and Outlook

# BACKGROUND

## □ The MOSAIK Project

The German Federal Ministry of Education and Research (BMBF), funded a joint project in 2016, named as Model-based city planning and application in climate change (MOSAIK) to develop an urban climate model within the framework of **Urban Climate Under Change ([UC]<sup>2</sup>)**.

## □ Main Aim

To develop a highly-efficient, state-of-the-art high-resolution microscale urban climate model that allows for building and turbulence-resolving simulations of large cities such as Berlin (Germany).

## □ PALM, the core Model

**PALM** (*Raasch and Schröter, 2001; Maronga et al., 2015*) was selected as the core model for the new microscale UC model named as PALM-4U of large cities such as Berlin (Germany).



1995: Prof. Siegfried Raasch! After his first successful PALM LES run.

# PALM, The LES Model.

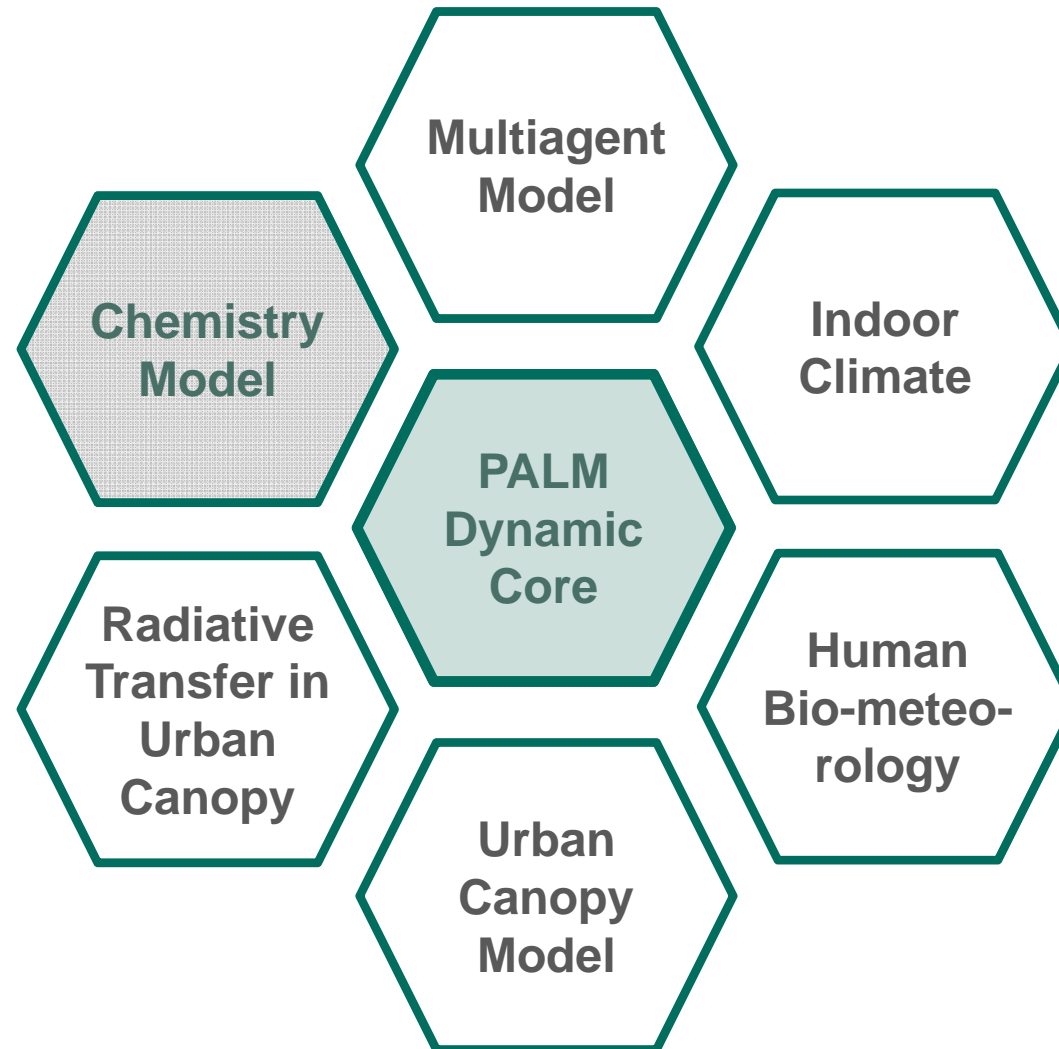
[Background]

- The PALM is based on the non-hydrostatic, filtered, incompressible Navier-Stokes equations in Boussinesq-approximated form.
- The Model has 6 prognostic quantities ( $u$ ,  $v$ ,  $w$ ,  $\theta$ ,  $q_v$  and an optional 's' for passive tracer).
- An additional equation for subgrid scale TKE 'e' (default **LES** mode) OR The total TKE (**RANS** mode).



Prof. Siegfried  
Raasch in 2018

- PALM-4U = PALM-LES + Urban Climatology + Air Chemistry



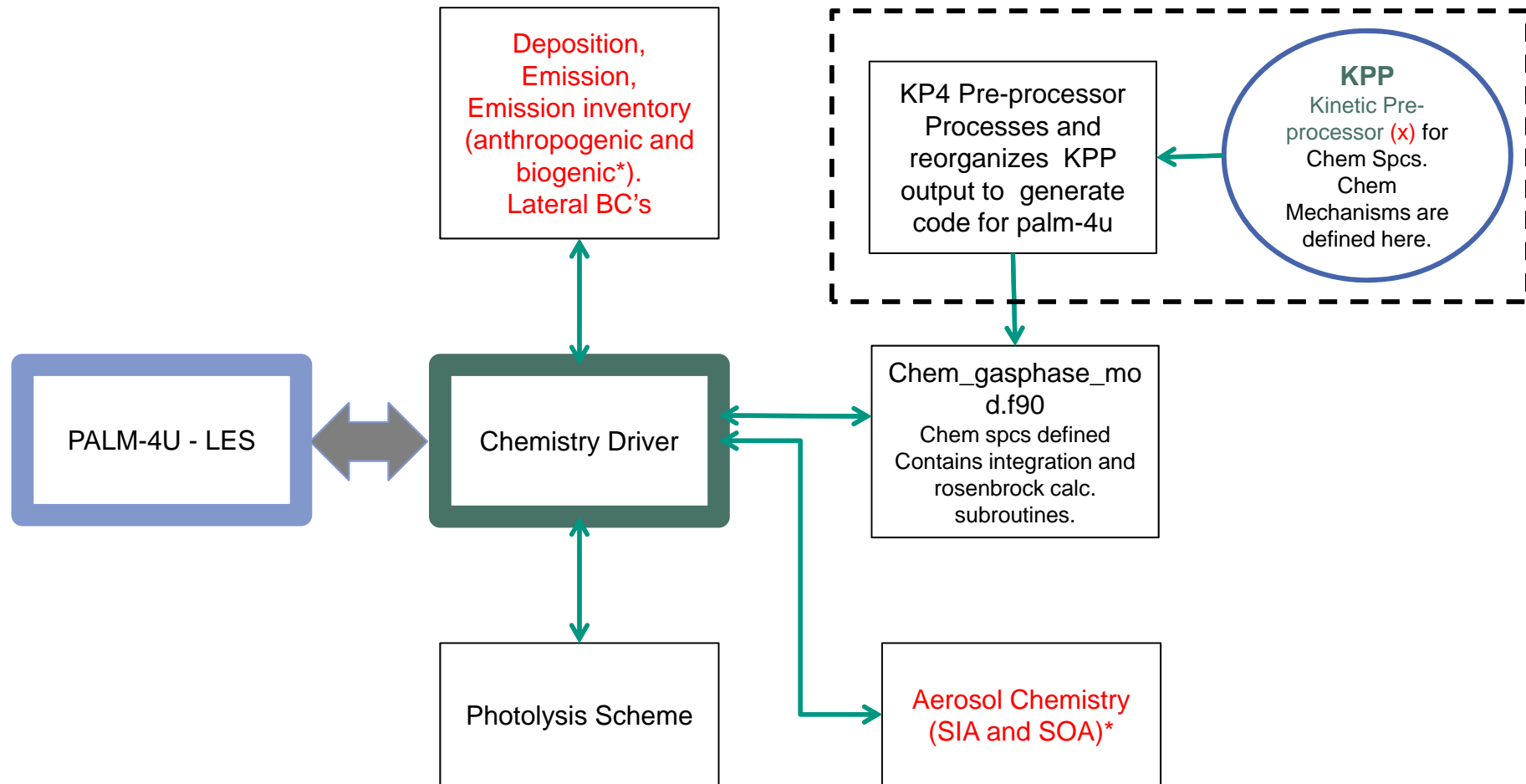
# CHEMISTRY IN PALM-4U

## PALM-4U! A Microscale Urban Climate & Air Quality Model ●●●●●



# Interface b/w Chemistry and PALM-4U

[Chemistry in PALM-4U]



\* Not implemented as yet

(x) Damian et al., 2002

<http://people.cs.vt.edu/asandu/Software/Kpp/>

## □ Current Features of Chemistry Model in PALM-4U Modeling System:

- An 'Online' coupled chemistry in LES mode for Gas-phase chemistry.
- Chemical reactions,
- Advection and diffusion
- Photolysis
- Ability to take any user provided chemical mechanism
- Passive tracer
- Nesting
- Static emissions in time and space.



# A Case Study from Downtown Berlin - Germany

## □ Model Setup

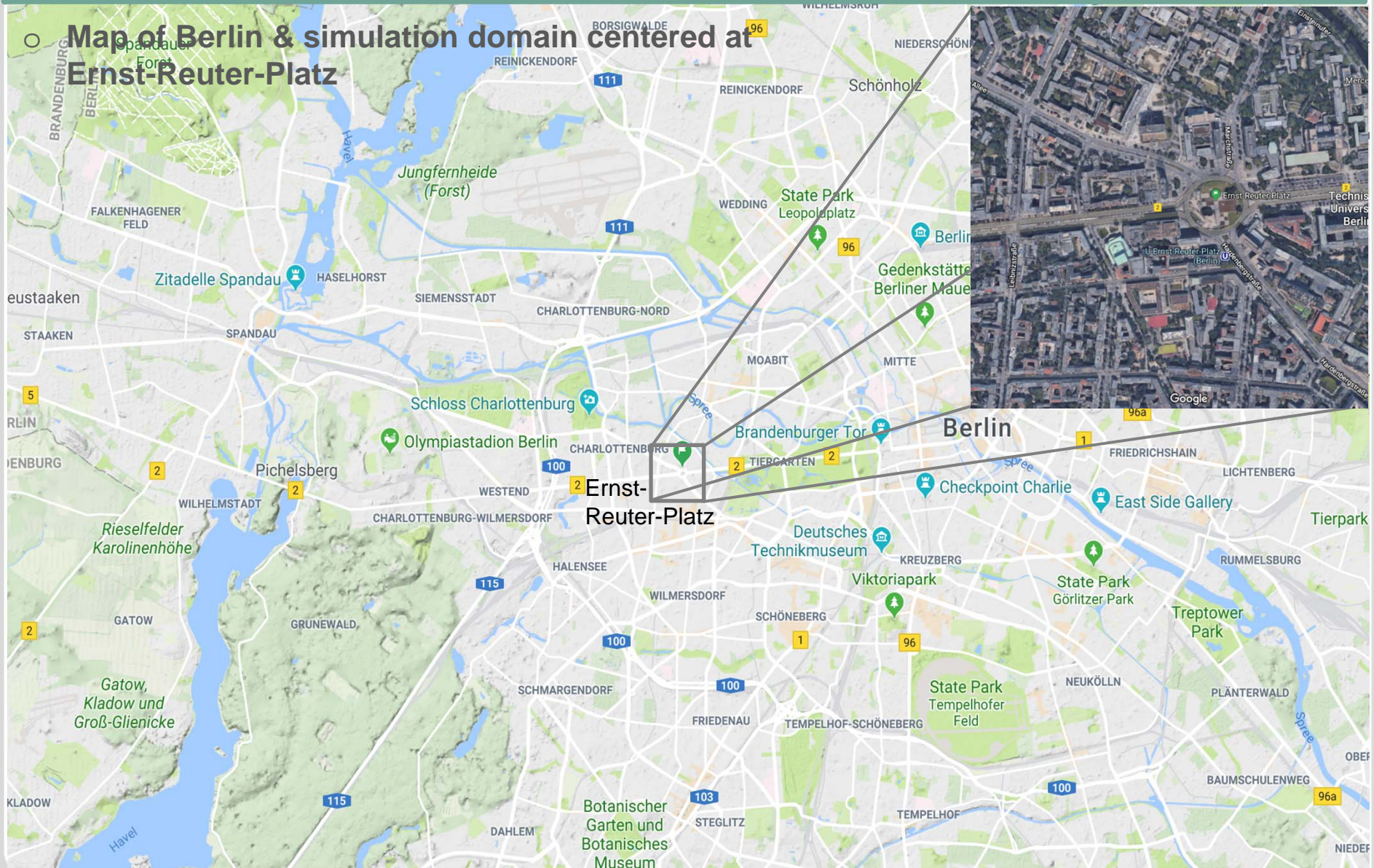
- $nX = nY = 96$ ,  $nZ = 120$ ;  $dX=dY=dZ = 10$  m;  $Ug = Vg = 1.0$  m s<sup>-1</sup>
- Day & Time: 21 July, 5:00 UTC; Simulation length = 6 hours.
- Modules: radiation, urban surface model, land surface model, canopy model, chemistry model, photolysis model
- Emissions related to OpenStreetmap street types:  
Enhancement factor for main roads = 01.667, Reduction factor for side roads = 0.334
- Emission: NO = 1.318 ppm s<sup>-1</sup>; NO<sub>2</sub> = 0.368 ppm s<sup>-1</sup>; RH = 0.1804 ppm s<sup>-1</sup>;  
PM10 = 0.75 ug m<sup>2</sup> s<sup>-1</sup>.

## □ The mechanism has 11 gas-phase chemical species and one non-reactive aerosol(PM10).

```
{1.} NO2 + hv = NO + O3           : phot(j_no2)
{2.} O3 + hv = 2OH + O2          : phot(j_o31d)
{3.} NO + O3 = NO2               : arr2( 1.8E-12_dp, 1370.0_dp, temp)
{4.} RH + OH = RO2 + H2O         : arr2( 2.E-11_dp, 500.0_dp, temp)
{5.} RO2 + NO = NO2 + RCHO + HO2 : arr2( 4.2E-12_dp, -180.0_dp, temp)
{6.} HO2 + NO = NO2 + OH         : arr2( 3.7E-12_dp, -240.0_dp, temp)
{7.} NO2 + OH = HNO3             : arr2(1.15E-11_dp, 0.0_dp, temp)
{8.} PM10 = PM10                 : 1.0_dp
```

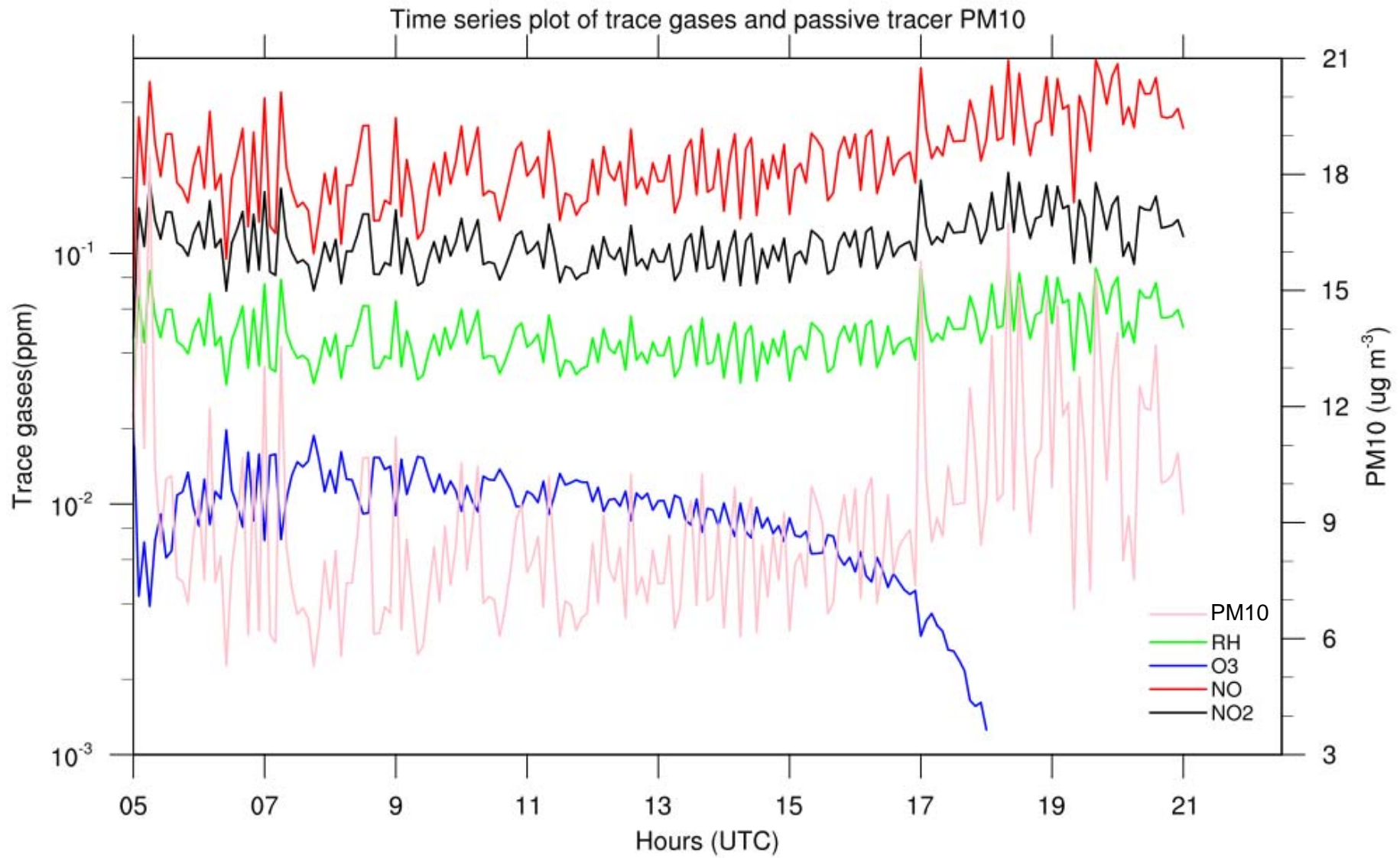
# Simulation Domain

[A Case Study-Berlin]



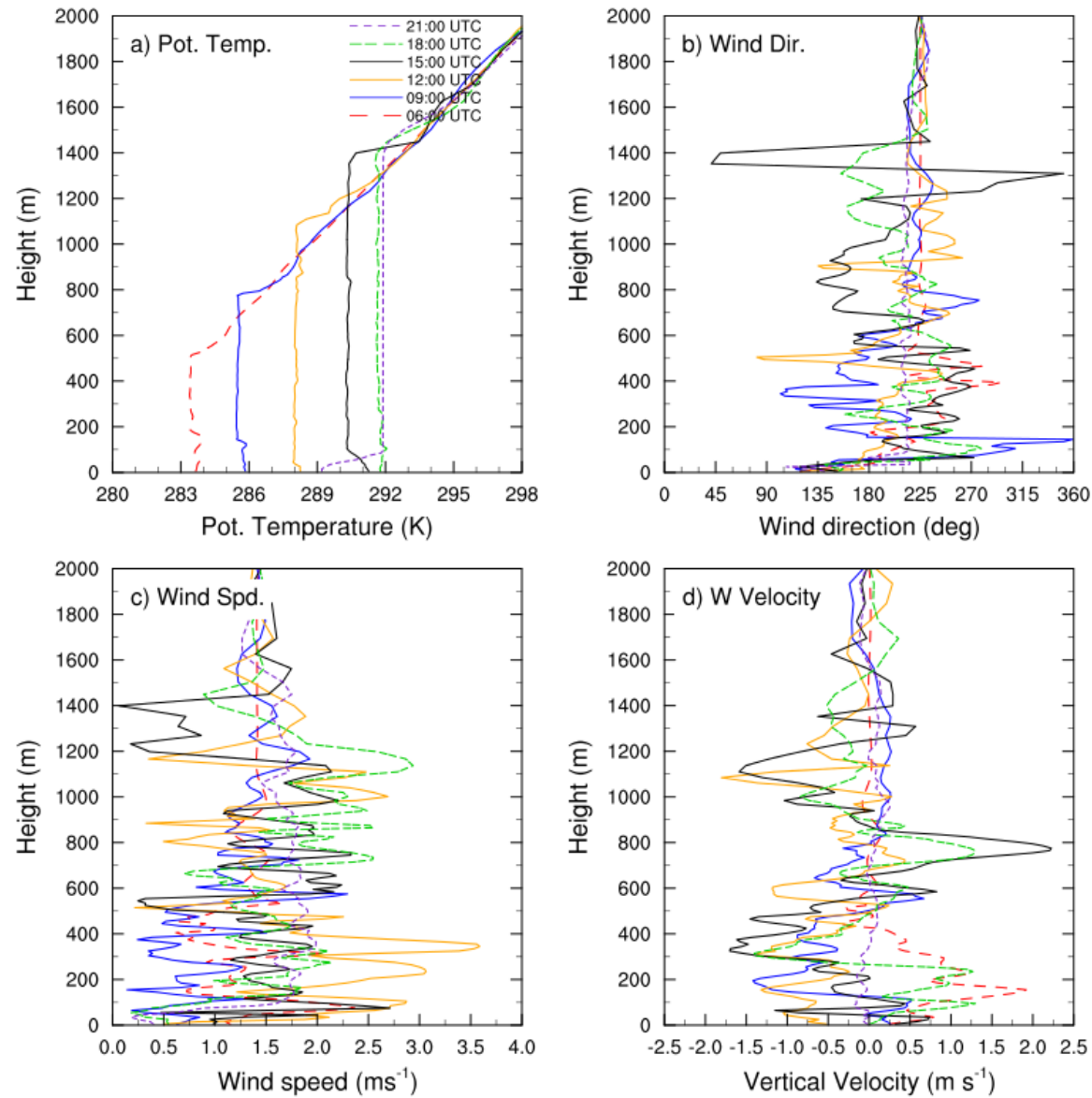
# Results

[A Case Study-Berlin]



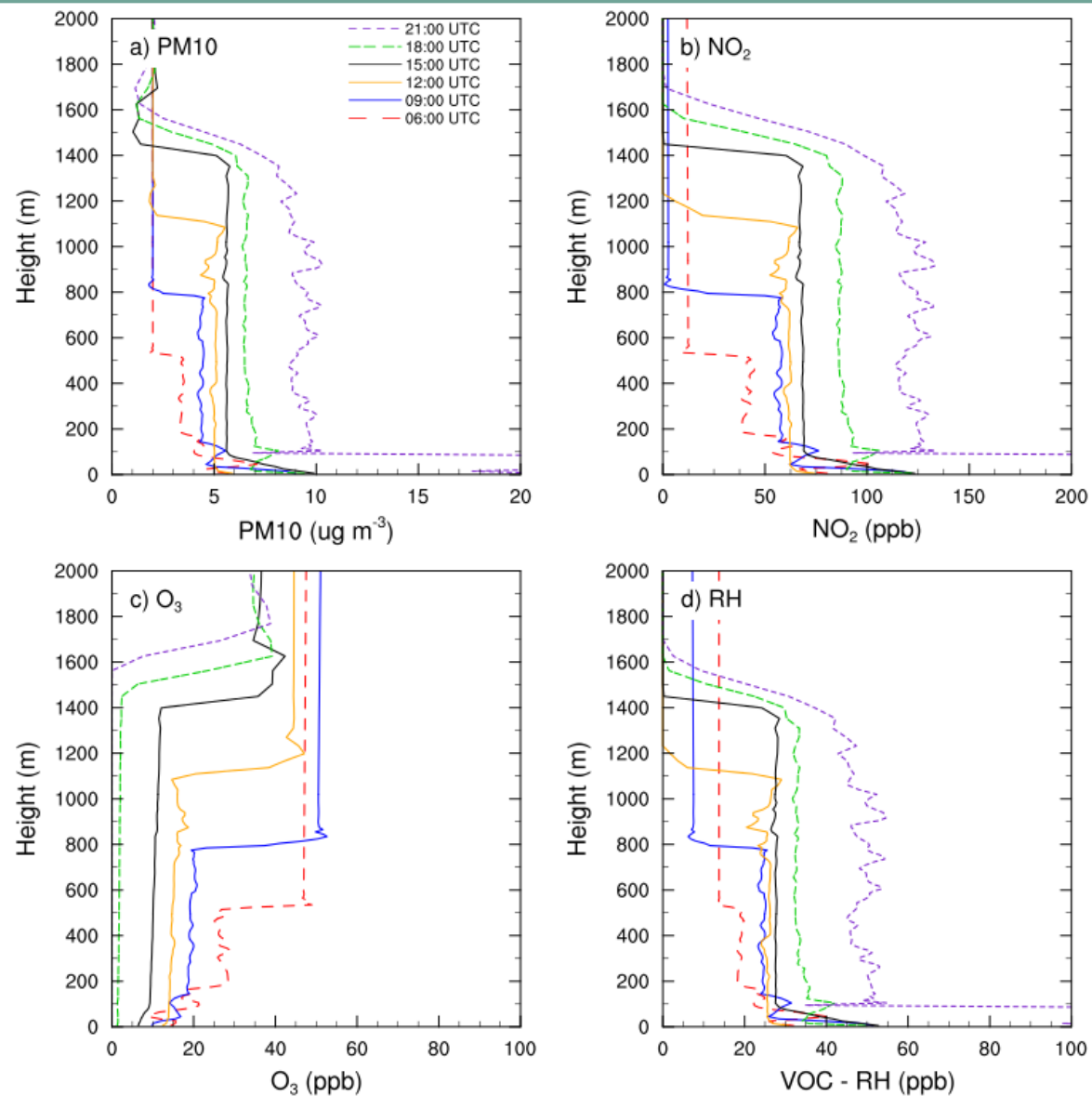
# Results

[A Case Study-Berlin]



# Results

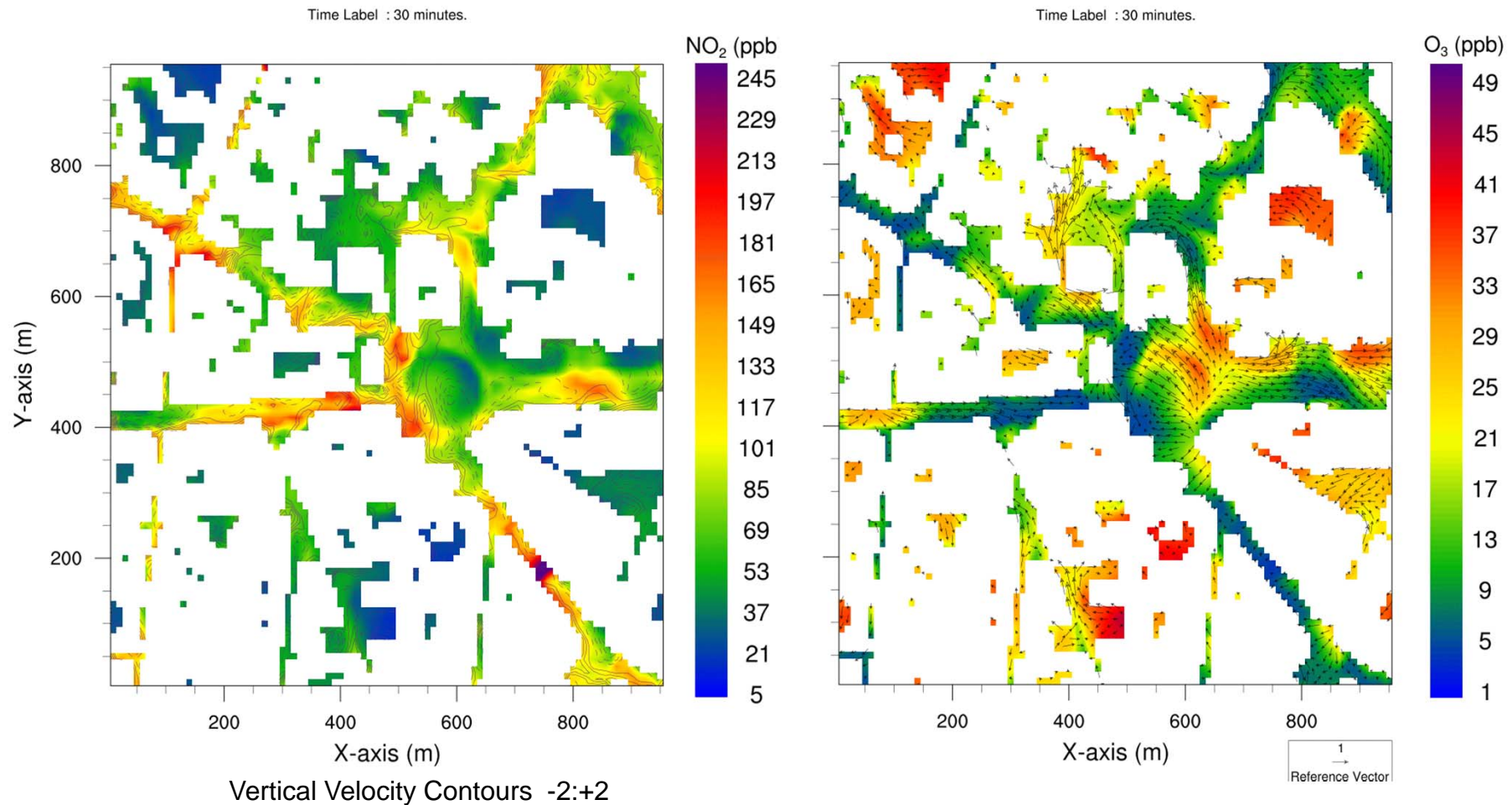
[A Case Study-Berlin]



# Results

[A Case Study-Berlin]

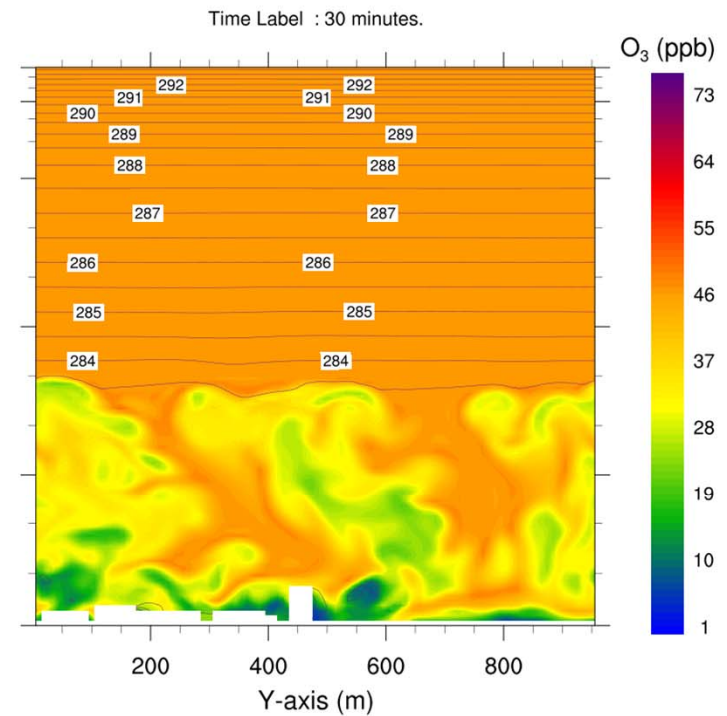
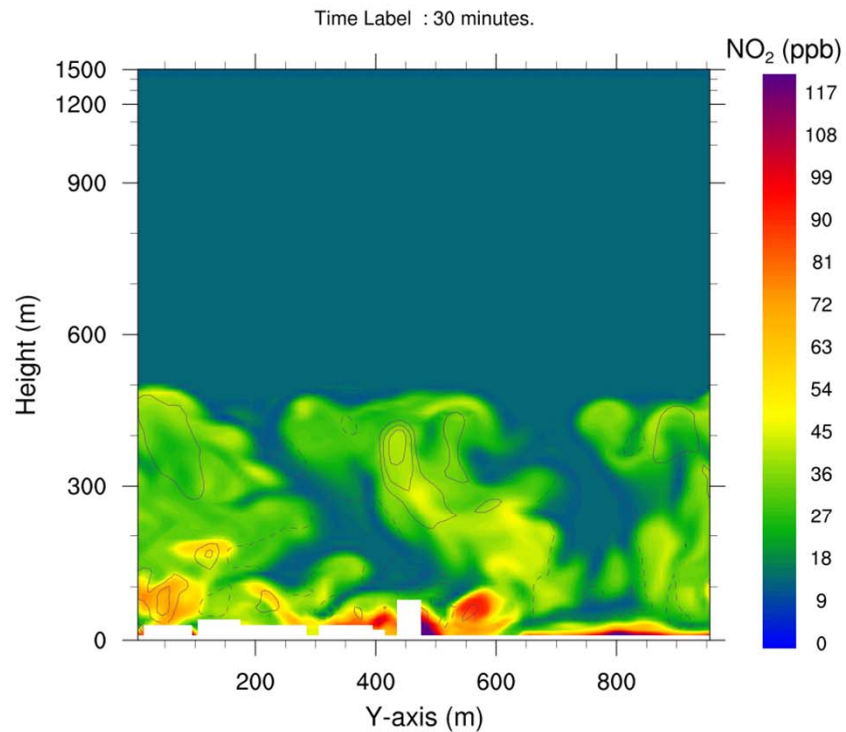
Horizontal cross-sections; Level: 5 meter; Left Panel: NO<sub>2</sub> shaded, W-Contours, Right Panel: O<sub>3</sub> shaded and horizontal wind vectors.



# Results

[A Case Study-Berlin]

Vertical cross-sections; Left Panel:  $\text{NO}_2$  shaded, W-Contours, Right Panel:  $\text{O}_3$  shaded, potential temperature contours.



# Summary and Outlook

## □ Summary

- Turbulence and building resolving LES PALM-4U model allows accurate simulation of advection, reaction, and deposition of atmospheric trace gases and aerosols at appropriate scale.
- PALM-4U is a potential candidate for the future state-of-the-art comprehensive urban climate modelling system that could be used for the assessment, prediction and investigation of urban climatology, air quality and city planning of large urban areas.

## □ Coming soon ...

- Chemistry forcing at the lateral boundaries of the parent domain
- Aerosol chemistry (SIA and SOA). SALSA sectional aerosol model (Kokkola et al., 2008) in the process to be incorporated in PALM-4U.
- Deposition module for chemical species and aerosols.
- Detailed anthropogenic emissions (temporal and spatial disaggregation, VOC split etc.).
- Reynolds Averaged, Navier-Stokes (RANS) Mode for larger domain, longer simulations and complex mechanisms.



# Wenn du Luft atmest, solltest Du Dich darum kümmern!

**Danke für die Aufmerksamkeit!**

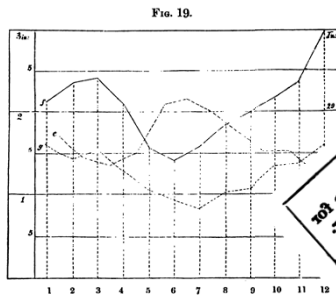
[basit.khan@kit.edu](mailto:basit.khan@kit.edu)

[renate.forkel@kit.edu](mailto:renate.forkel@kit.edu)

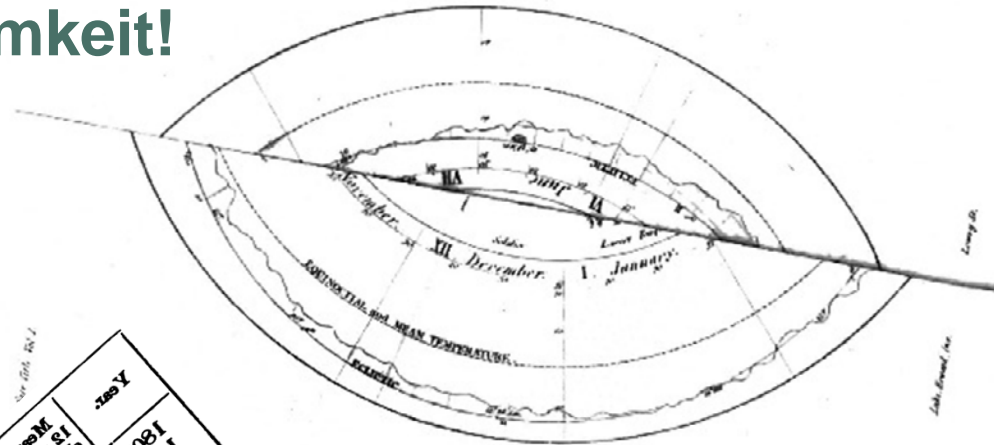
[matthias.mauder@kit.edu](mailto:matthias.mauder@kit.edu)

[sabine.banzhaf@met.fu-berlin.de](mailto:sabine.banzhaf@met.fu-berlin.de)

[emmanuele.russo@met.fu-berlin.de](mailto:emmanuele.russo@met.fu-berlin.de)



Year	1850	1851	1852	1853	1854	1855	1856	1857	1858	1859	1860	1861	1862	1863	1864	1865	1866	1867	1868	1869	1870	1871	1872	1873	1874	1875	1876	1877	1878	1879	1880	1881	1882	1883	1884	1885	1886	1887	1888	1889	1890	1891	1892	1893	1894	1895	1896	1897	1898	1899	1900
Mean of the Year	50.1	50.2	50.3	50.4	50.5	50.6	50.7	50.8	50.9	51.0	51.1	51.2	51.3	51.4	51.5	51.6	51.7	51.8	51.9	52.0	52.1	52.2	52.3	52.4	52.5	52.6	52.7	52.8	52.9	53.0	53.1	53.2	53.3	53.4	53.5	53.6	53.7	53.8	53.9	54.0	54.1	54.2	54.3	54.4	54.5	54.6	54.7	54.8	54.9	55.0	



THE  
**CLIMATE OF LONDON,**  
 DEDUCED FROM  
**Meteorological Observations,**  
 MADE IN THE METROPOLIS,  
 AND AT  
 VARIOUS PLACES AROUND IT.  
 BY LUKE HOWARD, GENT.  
 CITIZEN OF LONDON; HONORARY CITIZEN OF MAGDEBURG; FELLOW  
 OF THE ROYAL SOCIETY, AND HONORARY ASSOCIATE OF THE  
 SOCIETIES OF ARTS OF HAMBURG AND LEIPZIG.  
 FIRST EDITION,  
 PRINTED IN 1818.

