

## How good is the air we breathe?

### Modelling air quality in cities with PALM-4U – the impact of biogenic VOC and pollen

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#### In Short

- Air pollution is a serious environmental problem in urban areas that risks human health, quality of life and contributes towards climate change.
- PALM-4U including air chemistry coupled to a microscale urban climate model was developed as tool to assist planners and policy makers to formulate mitigation measures and adaptation strategies for cities.
- Evaluation, further development, enhancement and improvement in the air chemistry model of PALM-4U is underway.

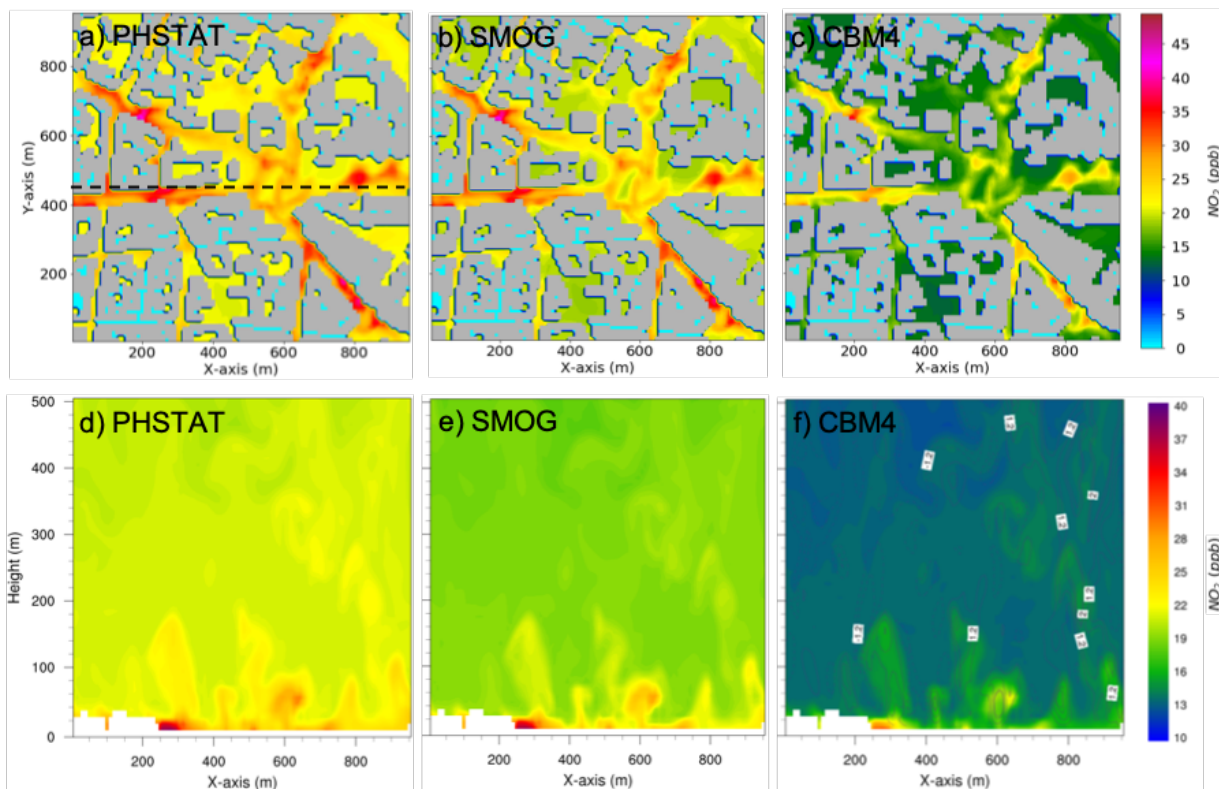
More than 96% of Europe's population is exposed to higher levels of at least one of the major air pollutants such as particulate matter,  $\text{NO}_x$  ( $\text{NO}_2 + \text{NO}$ ) and Ozone [1]. As the world become increasingly more urbanized, this makes urban conurbation vulnerable to environmental degradation and human health. The concentrated population in cities where largely natural landscape is replaced with human built artificial landscape, buildings and structures, leads to concentrated resource consumption, higher energy demand and deteriorated air quality. Hence, urban areas require serious attention. In particular air pollution has marked social, economic and environmental impacts leading to shorter life span, increased medical costs, reduced productivity, damage to terrestrial and marine eco-systems, a negative impact on biodiversity, deterioration of material, and reduced crops yield. In Europe only, air pollution is the number one environmental cause of premature death that is responsible for 400,000 deaths each year while the health related external costs range from 330 to 940 billion Euros per year [2].

Improved appreciation of emission, transport and chemical transformation of air pollutants is extremely important for developing effective mitigation policies and appropriate legislation to protect human and environmental health. Hence, detailed information about state of air quality of a given region is a prerequisite. In this regard, air quality models are useful tools that help identifying pollutant sources, sinks and hot-spots. The Ambient Air Quality Directive 2008, also encourages air quality modelling as one

of the means of performing air quality management tasks such as air quality assessment, forecasting and planning [3]. Large Eddy Simulation (LES) models have proven to be effective tools to simulate urban canopy features more accurately compared to Reynolds Averaged Navier-Stokes (RANS) models. Nevertheless, due to their high computational cost, LES models are so far barely applied for urban air quality studies.

In 2015, German Federal Ministry of Education and Research (BMBF), funded a joint project, MO-SAIK (Modellbasierte Stadtplanung und Anwendung im Klimawandel / Model-based city planning and application in climate change) within the framework of urban climate under change ( $[\text{UC}]^2$ ) initiative to develop a new state-of-the-art microscale urban climate model (UCM). The main aim of the MOSAIK project is to develop a user friendly urban climate model with unprecedented spatial resolution and computational efficiency that is able to represent the atmospheric processes in the urban canopy layer modified by anthropogenic activities and which constitute the urban microclimate [4]. The model aimed at allowing for microscale simulations of horizontal domains from 1000 to 2000  $\text{km}^2$ , with the ability to resolve turbulence and urban structures at a grid spacing  $\leq 10$  m. The highly parallelized and optimized large-eddy simulation (LES, turbulence resolving) model PALM [4], serves as the core for the new urban climate model (UCM) PALM-4U.

Representation of emission, dispersion, chemical transformation and removal of air pollutants in the urban canopy requires fine-scale turbulence-resolving simulations that can explicitly resolve building structures, surface heat fluxes at building facades, street canyons and terrain variations. A fully coupled 'on-line' gas-phase chemistry model has been implemented into PALM-4U. The model utilizes Kinetic PreProcessor KPP, Version 2.2.3 [6], to generate code for the numerical integration of the gas phase reactions. In a second preprocessing step the automatically generated code is optimized. Scalar as well as vector version of the chemistry code can be created. A choice between mechanisms of different complexities is possible. Aerosol processes are described by the sectional aerosol model [5]. The impact of urban features such as the urban heat island, ventilation in street canyons, and pollution hot-spots etc. on air pollution can be simulated. Due to the high computational demands of LES and chemistry models, a reduced chemistry mechanism was implemented which includes only major pollutants namely



**Figure 1:** Horizontal and vertical cross-sections of  $\text{NO}_2$  concentration at 1700 CET on 21st July, 2017, at Ernst-Reuter-Platz, Berlin, Germany, indicating differences in concentration patterns and magnitude of  $\text{NO}_2$  amongst three chemical mechanism. Black dashed line in figure 1a indicates location of the vertical cross-section.

$\text{O}_3$ ,  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{CO}$ , a highly simplified VOC chemistry and a small number of products. A full complex chemistry is available as well as strongly condensed mechanisms (Figure 1). Depending on the number of additional prognostic variables and the complexity of the mechanism the computational demand of an LES simulation with chemistry is about 2 to 10 times higher than for an LES simulation without chemistry. The model considers emissions from street canyons and selected point sources.

In the first phase MOSAIK-I, the chemistry model was developed, tested, and debugged. In the second phase MOSAIK-II, the main tasks include further development such as pollen, biogenic VOC emission, wet deposition, enhancement, validation and verification of the chemistry model using real world and wind tunnel measurements. Research work under this proposal will focus the idealized as well as validation studies of the chemistry model for larger urban areas under realistic meteorological conditions and chemistry boundary conditions. To undertake the desired task specially the validation and verification studies require substantial amount of computational resources. This work would help both palm development team as well as PALM users to improve, refine and extend the model as a scientific research tool as well as an aid for policy makers and administrators

to comply with air quality standards, and devise mitigation measures and adaptation strategies for urban planning and development.

#### WWW

<https://imk-ifu.kit.edu>

#### More Information

- [1] EEA, *Technical report. CSI 004*, 1-41 (2018a).
- [2] EC, *Technical report. IP/13/1274*, 1-3 (2013a).
- [3] Eur-Lex, *Technical report. 2008/50/EC*, 1-11 (2008).
- [4] B. Maronga et al., *Meteorologische Zeitschrift. 28(2)*, 105-119 (2019).
- [5] M. Kurppa et al., *Geoscientific Model Development. 12*, 1403–1422 2515?2551 (2019).
- [6] V. Damian, A. Sandu, M. Damian, F. Potra, and G.R. Carmichael, *Computers and Chemical Engineering. 26(11)*, 1567–1579 (2002).

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