

How good is the air we breathe?

Modelling air quality in cities with PALM-4U – the impact of biogenic VOCs 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.
- An air chemistry model has been developed as part of PALM-4U (i.e PALM for urban applications) components that are added to an LES model PALM to assist planners and policy makers to monitor air quality, formulate mitigation measures and adaptation strategies for cities.
- The chemistry model is continuously being evaluated, enhanced, improved and extended by addition of urban air chemistry applications that include aerosol, biogenic, and pollen emission modules.

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, 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 large resource consumption, higher energy demand and deteriorated air quality. In particular air pollution has marked social, economic and environmental impacts. In Europe only, air pollution is the number one environmental cause of premature death that is responsible for 400,000 deaths each 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 health and environment. 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].

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 ([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 aims at allowing for microscale simulations of horizontal domains from 1000 to 2000 km^2 , with the ability to resolve turbulence and urban structures at a grid spacing ≤ 10 m. To address this demand, the well established large eddy simulation (LES) model PALM has been enhanced by adding new components, including also transport and chemical transformation of pollutants, for urban applications named PALM-4U [5, 6]]. 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.

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 'online' gas-phase chemistry model has been implemented into PALM-4U. The model utilises Kinetic PreProcessor KPP, Version 2.2.3 [7], to generate code for the numerical integration of the gas phase reactions. In a second preprocessing step the automatically generated code is optimised. Scalar as well as vector version of the chemistry code can be created.

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. A choice of mechanisms with different complexity is available and can be further extended by the user. Strongly reduced chemistry mechanisms which include only major pollutants namely O_3 , NO , NO_2 , CO , and highly simplified VOC chemistry and as well as a full complex chemistry are available.(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

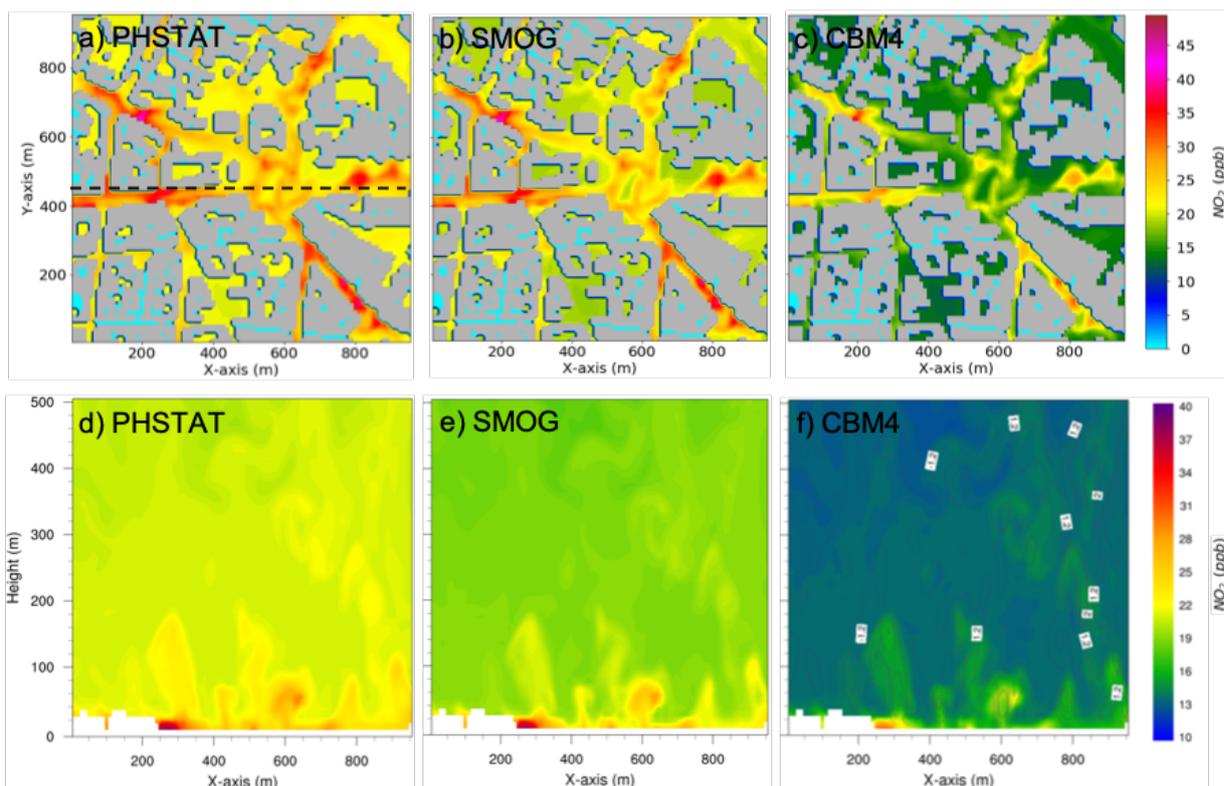


Figure 1: Horizontal and vertical cross-sections of NO_2 concentration at 1700 CET on 21st July, 2017, at Ernst-Reuter-Platz, Berlin, Germany, indicating differences in concentration patterns and magnitude of NO_2 amongst three chemical mechanism. Black dashed line in figure 1a indicates location of the vertical cross-section.

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 and tested [6]. In the second phase MOSAIK-II, the main tasks include further development such as pollen, biogenic VOC emissions, wet deposition, enhancement, validation and further verification of the chemistry model using real world and wind tunnel measurements. Research work under this proposal will focus on the idealised 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 a substantial amount of computational resources. In particular the investigation of the impact of biogenic VOC emissions from urban vegetation requires the application of sufficiently complex chemistry mechanisms with a corresponding computational demand.

This work will 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.

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

More Information

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