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Modelling the urban air quality in Hamburg with the new city-scale chemistry transport model CityChem

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Air quality modelling plays an important role by providing guidelines for efficient air pollution abatement measures. Currently, most urban dispersion models treat air pollutants as passive tracer substances or use highly simplified chemistry when simulating air pollutant concentrations on the city-scale. The newly developed urban chemistry-transport model CityChem has the capability of modelling the photochemical transformation of multiple pollutants along with atmospheric diffusion to produce pollutant concentration fields for the entire city on a horizontal resolution of 100 m or even finer and a vertical resolution of 24 layers up to 4000 m height. CityChem is based on the Eulerian urban dispersion model EPISODE of the Norwegian Institute for Air Research (NILU). CityChem treats the complex photochemistry in cities using detailed EMEP chemistry on an Eulerian 3-D grid, while using simple photo-stationary equilibrium on a much higher resolution grid (receptor grid), i.e. close to industrial point sources and traffic sources. The CityChem model takes into account that long-range transport contributes to urban pollutant concentrations. This is done by using 3-D boundary concentrations for the city domain derived from chemistry-transport simulations with the regional air quality model CMAQ. For the study of the air quality in Hamburg, CityChem was set-up with a main grid of 30×30 grid cells of 1×1 km^2 each and a receptor grid of 300×300 grid cells of 100×100 m^2. The CityChem model was driven with meteorological data generated by the prognostic meteorology component of the Australian chemistry-transport model TAPM. Bottom-up inventories of emissions from traffic, industry, households were based on data of the municipality of Hamburg. Shipping emissions for the port of Hamburg were taken from the Clean North Sea Shipping project. Episodes with elevated ozone (O_3) were of specific interest for this study, as these are associated with exceedances of the World Health Organization (WHO) guideline concentration limits for O_3 and of the regulatory limits for NO_2. Model tests were performed with CityChem to study the ozone formation rate with simultaneous variation of emissions of nitrogen oxides (NO_x) and volatile organic compounds (VOC). Emissions of VOC in urban areas are not well quantified as they may originate from various sources, including solvent usage, industry, combustion plants and vehicular traffic. The employed chemical mechanism contains large uncertainties with respect to ozone formation. Observed high-O_3 episodes were analyzed by comparing modelled pollutant concentrations with concentration data from the Hamburg air quality surveillance network (http://luft.hamburg.de/). The analysis inspected possible reasons for too low modelled O_3 in summer such as missing emissions of VOC from natural sources like green parks and the vertical exchange of O_3 towards the surface.