



# Validation of the air chemistry of PALM-4U using mobile measurements

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## Motivation

The validation of a model is an integral part of the quality assurance of model development. In our case, we validated the air chemistry using the VALM04 model run in Stuttgart. The chemistry here consists of a simple photostationary equilibrium. The boundary conditions were taken from the COSMO WRF model, into which the parent and the two child model domains were nested.

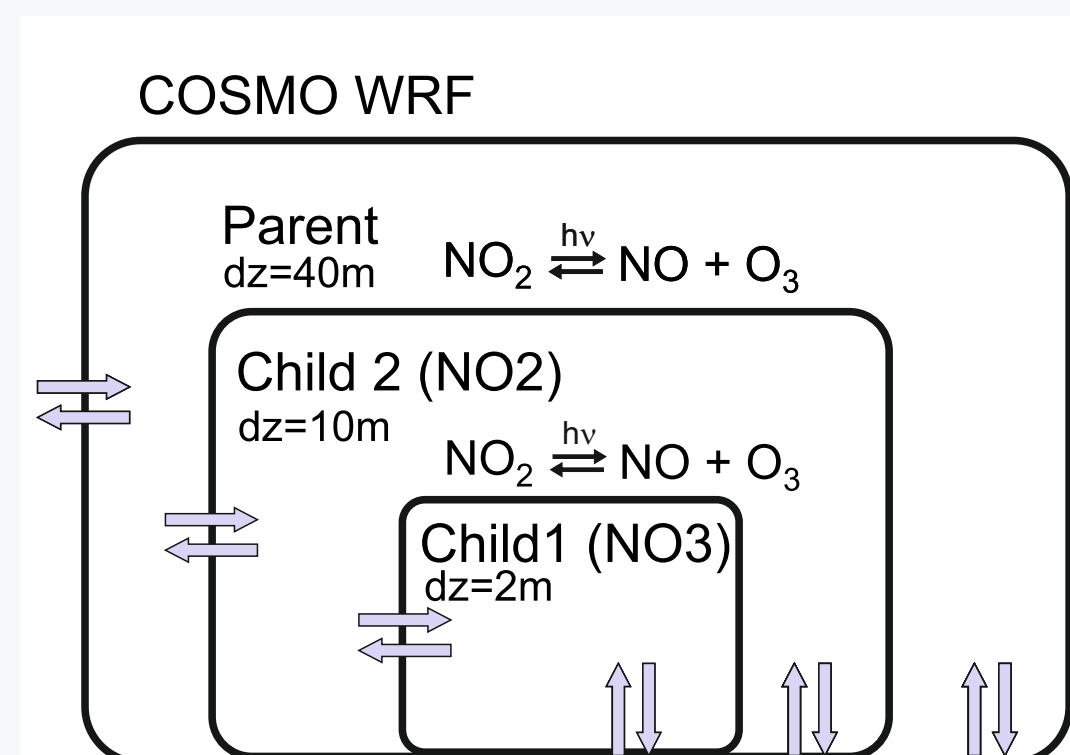


Figure 1: Schematic setup of the VALM04 simulation

## Measurement Setup

The simulation period was two days in 2018, during which we probed the Stuttgart valley with the MobiLab mobile laboratory and the DLR Cessna, which flew at different altitudes above Stuttgart. Both platforms were used to acquire data on the distribution of trace gases.



Figure 2: Cessna with MobiLab during an intercomparison.

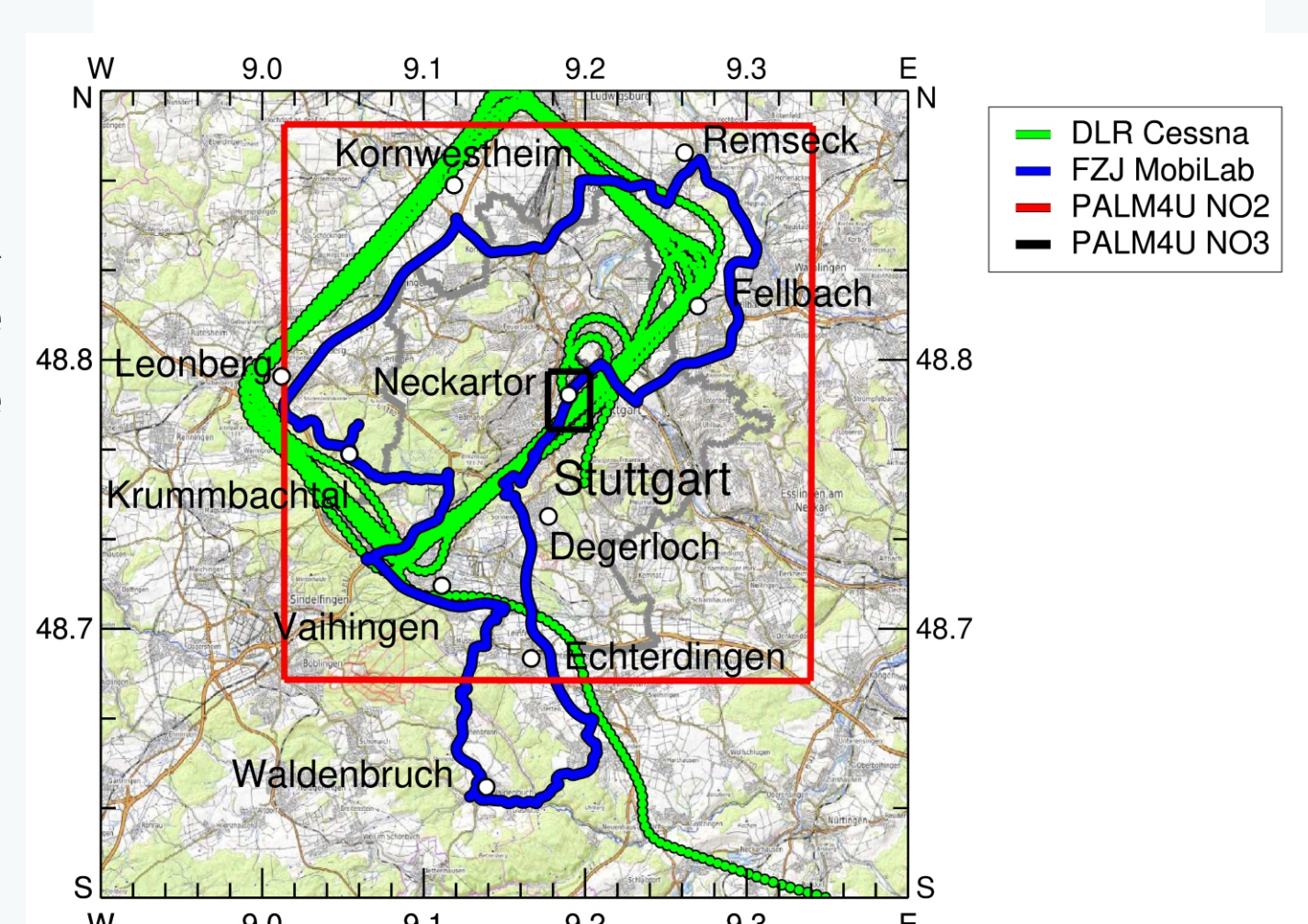


Figure 3: Tracks of Cessna and MobiLab within the different domains of the model region.

## Cessna measurements

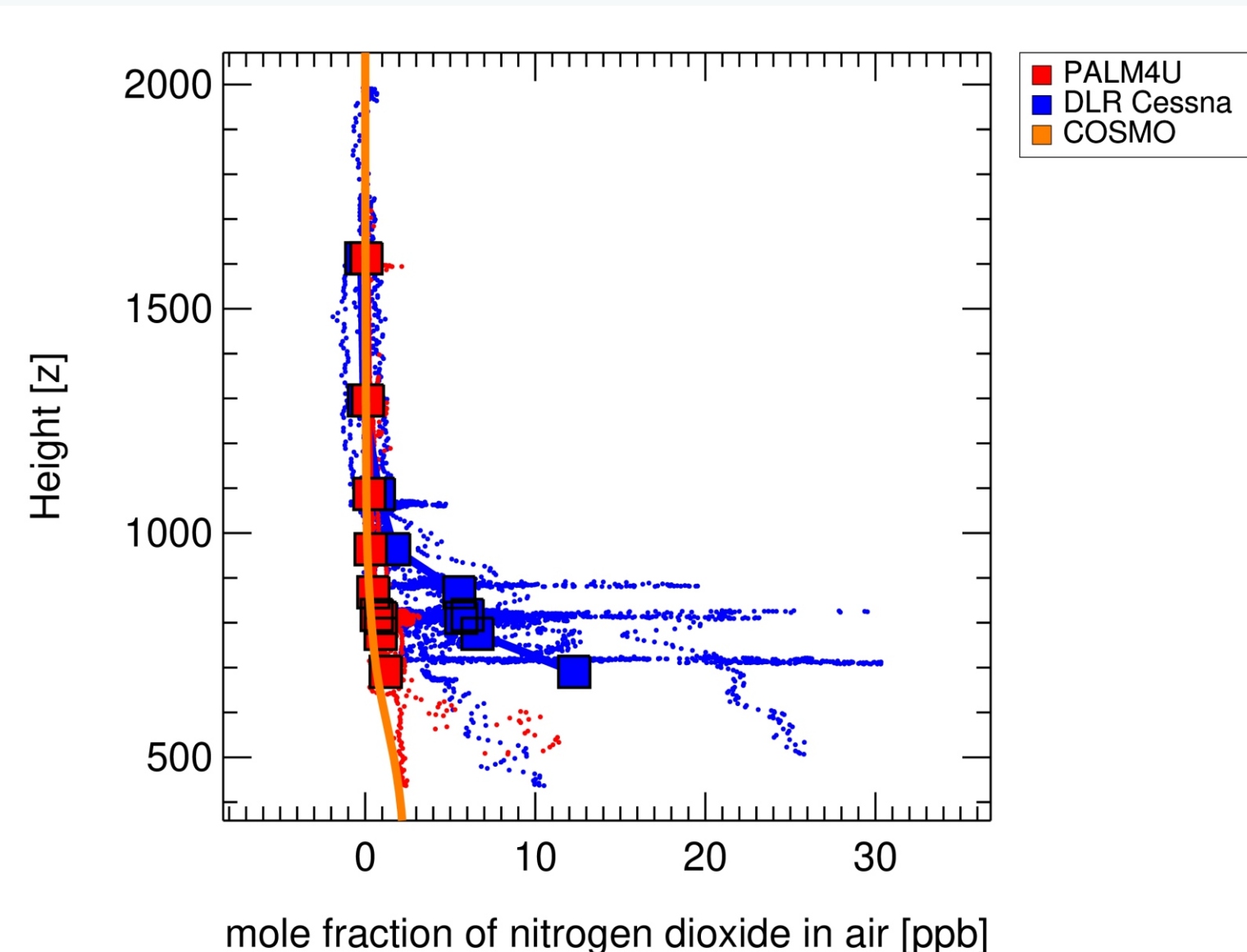


Figure 4: Measured (blue) and simulated (red) mole fraction of NO<sub>2</sub> at different heights. The orange line indicates the limiting mixing ratio as imposed by COSMO WRF. Simulated for child 1 domain for 2018/07/09 from 07:00 to 10:00.

Aircraft measurements provide an overview of the vertical distribution of trace substances. In general, the simulated and measured NO<sub>2</sub> values agree well at high altitudes. At lower altitudes, however, the model underestimates the observed NO<sub>2</sub> values because either the NO<sub>x</sub> source is too small overall or NO<sub>x</sub> is not transported upwards fast enough. This is also confirmed by the agreement of the simulated NO<sub>2</sub> with the NO<sub>2</sub> boundary value of COSMO-WRF.

The ozone mixing ratio of the model is also strongly influenced by COSMO-WRF (Figure 5). Here, the too low input values for ozone in COSMO-WRF lead to an underestimation also in PALM4U, while the Cessna data also agree with the ground site observations.

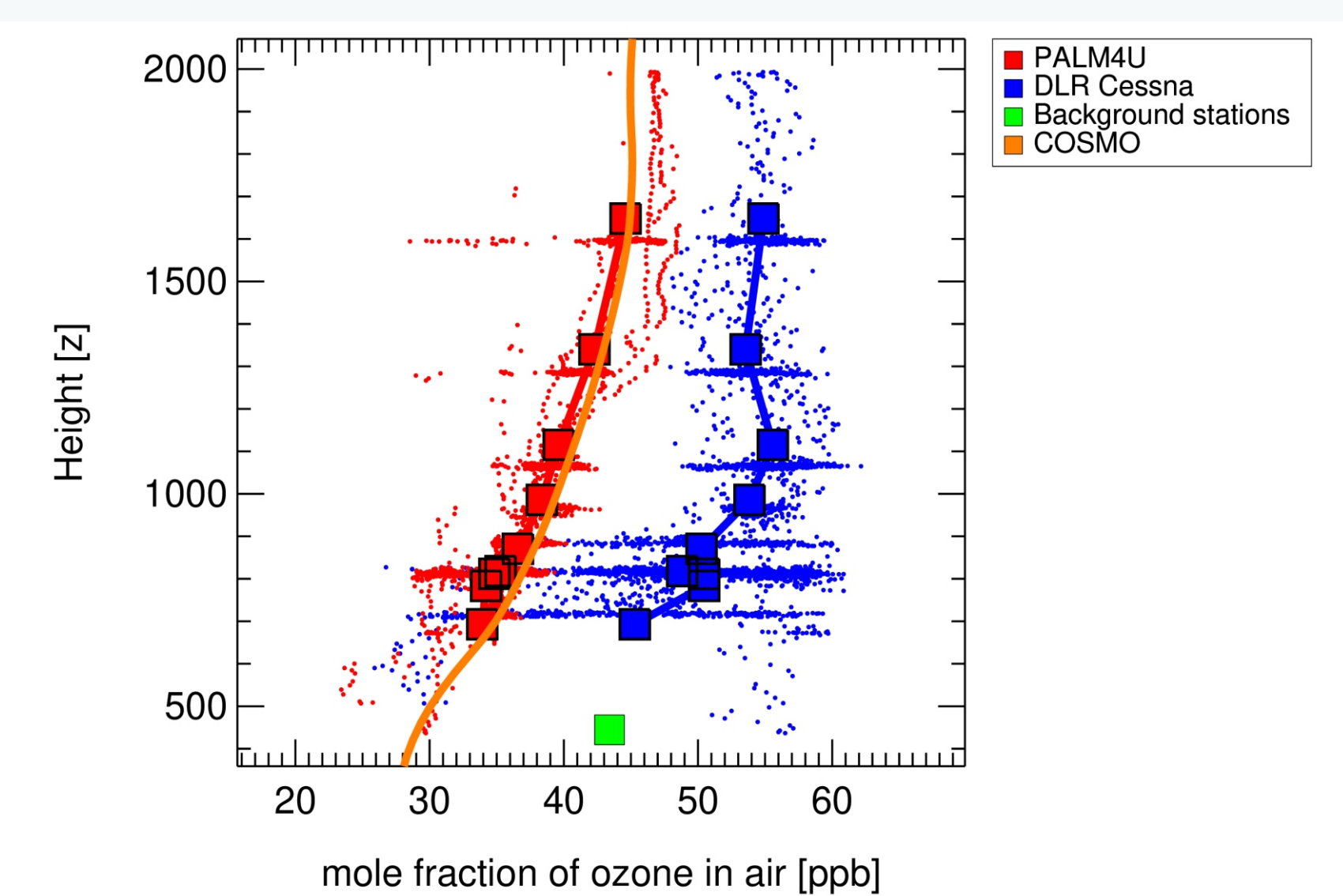


Figure 5: Measured (blue) and simulated (red) mole fraction of ozone at different heights. The orange line indicates the limiting mixing ratio as imposed by COSMO WRF. Simulated for Child 1 domain for 2018/07/09 from 07:00 to 10:00.

## MobiLab Measurements

The comparison of the measured and simulated data shows that the spatial distribution of the pollutants is well reproduced by the model. The decrease in nitrogen oxide concentrations north and south of Stuttgart corresponds to the observations. However, the increased concentrations on the A81 northwest of Stuttgart are not well represented in the model, possibly because the traffic density from the traffic flow model is too low here. Overall, the concentrations are too low due to the low resolution of 40 m in the parent model domain used here.

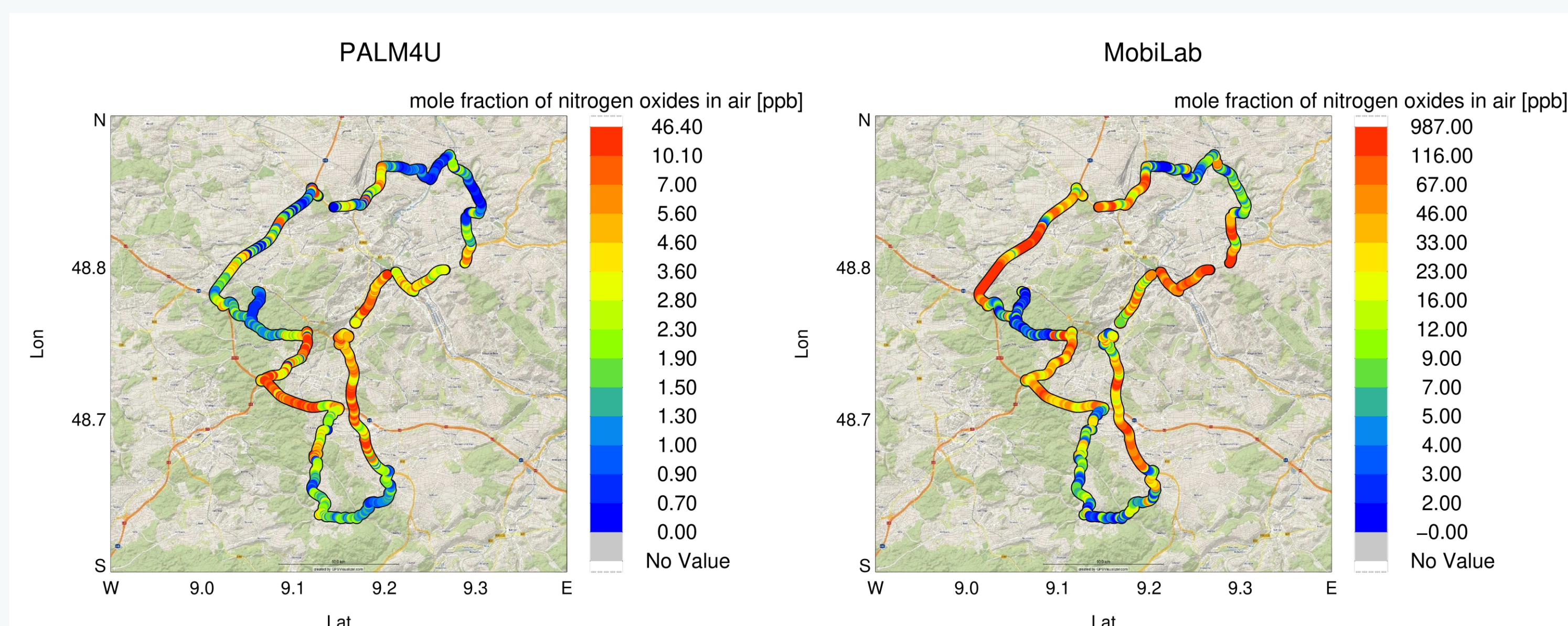


Figure 6: Simulated (left) and observed (right) mixing ratios of nitrogen oxide for the parent domain or 2018/07/08 from 10:57 to 14:04. The color denotes the respective amount fraction.

## Comparison at high resolution

Increasing the resolution from 40 m to 1 m improves the agreement between measurement and model. Although the distribution of simulated and measured values agrees, the model underestimates the observation by a factor of three, which is consistent with the comparison of the aircraft data. A refinement of the traffic model data could further improve the agreement.

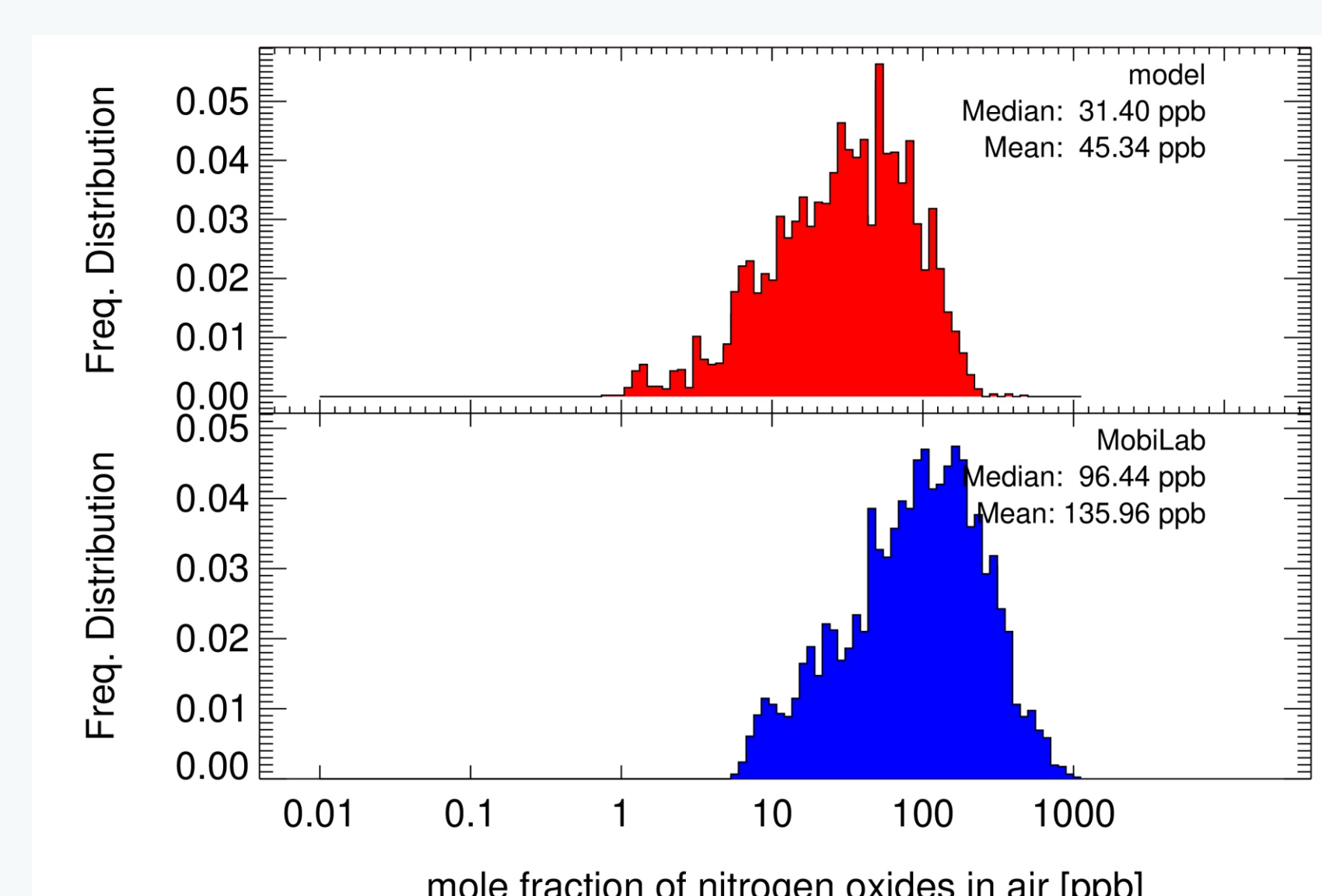


Figure 7: Frequency distribution of simulated (top) and measured (bottom) NO<sub>x</sub> mixing ratio for the domain with the highest spatial resolution of 1 m.