Project: 1234

Project title: Air Quality: Worldwide Analysis and Forecasting of Atmospheric Composition for Health (AQ-WATCH): High-resolution air quality multi-model forecast system for focus regions in Asia and the Americas

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For the AQ-WATCH project, the Environmental Modeling Group of Max Planck Institute for Meteorology is responsible for setting up a high-resolution air quality multi-model forecast system for the focus regions in Asia and the Americas in the AQ-WATCH project. Over the last report year, the Groups operated forecasted over China, Chile and Brazil with the regional chemical transport model Weather Research and Forecasting model coupled with Chemistry (WRF-Chem). It also set up an automation system to harmonise and coordinate the forecast data provided by different forecast models of the Group and other AQ-WATCH partners. The next-generation atmospheric chemistry model MUSICA (Multiscale Infrastructure for Chemistry and Aerosols) [1] was also installed and tested on the Levante system, which will contribute to the forecast system in the next report year.

For the forecasts over China, efforts have been made to downscale the emission input data to improve the mdoel performance. Emissions from inventory CAMS-GLOB-ANT-v4.2-R1.1 [2] with a resolution of 10 kilometers are downscaled into 1 kilometer by applying weight factors derived from various proxies, which are datasets correlated to individual emission sources (see Figure 1). Two model runs are designed with a regional model WRF-Chem to test the sensitivity of model simulation of pollutants (e.g. NO<sub>2</sub> and O<sub>3</sub>) to the original (control run) and downscaled emission (test run). The simulation fed with downscaled emissions gives lower biases of NO<sub>2</sub> and O<sub>3</sub> compared with control run. Figure 2b shows the difference of NO<sub>2</sub> simulations between control and test run under stagnant condition (low wind speed). On 9 out of 12 environmental observation sites (green triangles in Figure 2a), overestimations in simulated NO<sub>2</sub> in the control run are reduced in test run. It shows that the change of emission flux does not only affect the simulated concentrations at the emission spots but also in the downwind areas.

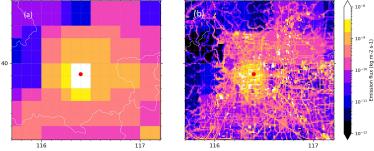
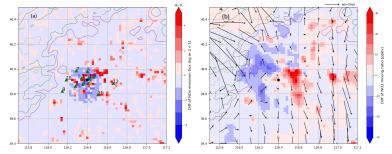


Figure 1. Emissions flux of nitrogen oxides (NOx) in CAMS-GLOB-ANT-v4.2-R1.1 (original emission inventory) (left) and downscaled emissions in this study (right) in Beijing city (red dot represents Beijing city center).



**Figure 2.** Difference of NOx emissions flux between original and downscaled emissions (left); difference of NO2 mixing ratio simulated in control run and test run at 16:00, January 19, 2019. (right; black dots mark Beijing city center; three terrain height contour lines plotted with values 250m (purple), 500m (green) and 1000m (yellow); wind field plotted with scaled black arrows)

For the forecasts in South America, the daily air quality forecasts in Chile are performed with the WRF-Chem model (10 km resolution) for the next three days. The same model is used for the forecasts in Brazil. Seven variables are analyzed, including five trace gases (CO, NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub> and O<sub>x</sub>) and aerosols (PM<sub>2.5</sub> and PM1<sub>0</sub>). The levels of fine (PM<sub>2.5</sub>) and coarse (PM<sub>10</sub>) aerosols are assessed against the Santiago measurement network (Figure 3 top panel). In addition, the global forecasts made at NCAR and ECMWF are compared to illustrate the improvements in model performance with the high resolution of the regional

forecasts. Nevertheless, the averaged diurnal variation (Figure 3 bottom panel) of the PM<sub>10</sub> concentration is too large for all forecasts. This discrepancy is under investigation.

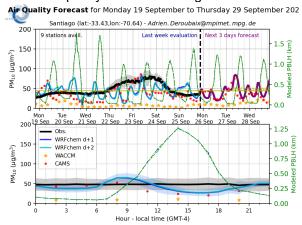


Figure 3. Example of the forecast in Chile with the regional WRF-Chem model (top) and its comparison with global models and observations (bottom)

The model outputs from these forecasts and the other forecasts by the AQ-WATCH partners are harmonised and coordinated to deliverer a multi-model ensemble forecast. Near real-time evaluation of the forecast data using local observational datasets area also performed in the forecast system. The ensemble mean and the model evaluation with observations are shown daily on the AQ-WATCH Toolkit (Figure 4(a) & (b)), a web-interface developed by the project as a user-friendly product to provide air quality information. A fully connecting network is used through the machine learning (ML) workflow MLAir (Machine Learning on Air data; [3]) to generate a ML-driven ensemble based on bias correction from observational data (see Figure 4(c) & (d)), which will contribute to the AQ-WATCH multi-model forecast system upon further development in the next report year.

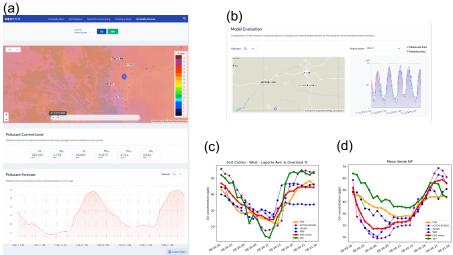
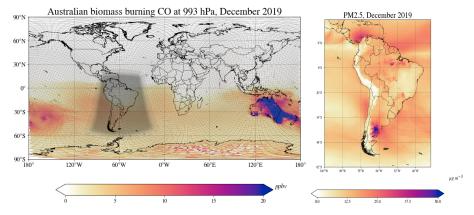


Figure 4: AQ-WATCH Toolkit Air quality forecast module: Map of predicted concentrations (ensemble mean) over Colorado and its variation over the last week at the selected location (a) and the model evaluation panel (b). Time series of the individual regional models, ensemble mean and the prediction from MLAir on August 20, 2022 (c & d). Panel d shows a case where the ML-driven ensemble (FCN; orange line) can show improvements over other models when the regional chemical transport models do not predict the observed concentration (green line) well.

MUSICA, the next generation community infrastructure for studying atmospheric chemistry across all scales with a zooming capability in a unified and modular approach developed by NCAR, was also installed and tested in the Levante system. Global simulations using the model MUSICAv0 [1] with local refinement over South America where performed, using a resolution of ~111km in the global domain, that where refined to ~28km over the aforementioned subcontinent for the year 2019, using a CO tracer for biomass burning from Sub-Saharan Africa, the Amazon, Southern South America and Australia (Figure 5 left panel). The results, which are compatible with previous observations, are promising in terms of forecasting regional and long-range air pollution events, while still allowing for a high-enough resolution to analyse local effects (see Figure 5 right panel). With further testing and development, MUSICA will also contribute to the AQ-WATCH multimodel forecast system in the next report year.



**Figure 5**: Simulation of mean global effect of Australian Biomass burning in December 2019 in a grid with South American refinement by MUSICA using a CO-like tracer (left). Monthly mean for PM2.5 at a regional scale in the same month (right).

## References:

- 1. Schwantes, R.H., et al., Evaluating the Impact of Chemical Complexity and Horizontal Resolution on Tropospheric Ozone Over the Conterminous US With a Global Variable Resolution Chemistry Model. Journal of Advances in Modeling Earth Systems, 2022. **14**(6): p. e2021MS002889.
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- 3. Leufen, L.H., F. Kleinert, and M.G. Schultz, *MLAir* (v1.0) a tool to enable fast and flexible machine learning on air data time series. Geosci. Model Dev., 2021. **14**(3): p. 1553-1574.