Project report

Project: **1170**

Project title: **Atmospheric greenhouse gases and the Carbon cycle (AtmoC)**

Principal investigator: **André Butz**

Report period: **2023-07-01 to 2024-06-30**

WP1: WRF-Chem simulations: Modelling CO2 and fossil fuel tracer concentration fields in urban hotspots

For five urban metropolitan areas in Germany (Berlin, Rhine-Ruhr metropolitan region, Rhine-Neckar metropolitan region, Nuremberg, and Munich) we have simulated the CO2 enhancements on 1km resolution using the Weather Research and Forecasting (WRF)- Model and utilizing the optimized simulation parameters, which were earlier investigated (see last project report). To obtain a concentration record, it was necessary to align existing emission inventories with the required grid and consider the temporal development of the flows. For biogenic emissions, we utilized the Vegetation Photosynthesis and Respiration Model (VPRM) with a spatial resolution of 1 km and a temporal resolution of 1 hour. Fossil emissions were extracted from the TNO inventory (Emissions (tno.nl)), which is available at a 1 km resolution and reports a diurnal cycle of emission factors. Various tracers (fossil CO2, biogenic CO2, biofuel CO2, traffic CO2, and fossil CO) were simulated at a 1 km resolution for the entire year 2018. The data was submitted as Deliverable (D.12.1) within the ITMS-M project and has been shared with colleagues from the ICOS project as well. Since a realistic simulation is crucial for the execution of the planned experiments on observation strategies, the simulated CO2 increases were compared with measured CO2 increases at the ICOS station Gartow (see Fig.1 for the comparison in winter 2018). Excellent agreements were found for winter, summer, and autumn. In spring, larger deviations were detected, likely attributable to inaccuracies in the VPRM emissions during the spring.

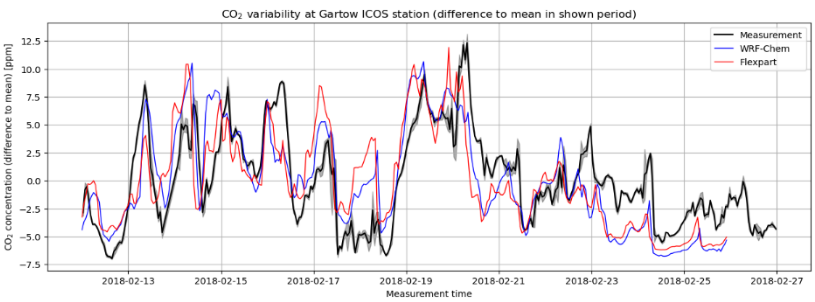

Fig 1: Comparison of CO2 enhancement from measurements (black), WRF-Chem simulations (blue) and Flexpart simulations (red) at station Gartow.

WP2: Flexpart-WRF Simulations: Inversion of fossil fuel CO2 in urban hotspots

At the beginning of 2023, the Lagrangian model Flexpart-WRF was set up to calculate the footprints of the stations. The simulated WRF meteorological data are used as drivers. A station comparison was also carried out for Flexpart-WRF, allowing both models (WRF-Chem and Flexpart-WRF) to be compared with each other and with the measured concentration increases (see Fig.1). We next used an inverse framework and examined initial observation strategies in Berlin. In a prototypical setup, an inversion of fossil emissions as well as total emissions in Berlin was performed for a period of 2 weeks (see Fig. 2). The corresponding code is freely available and published (Maiwald and Luken-Winkels,

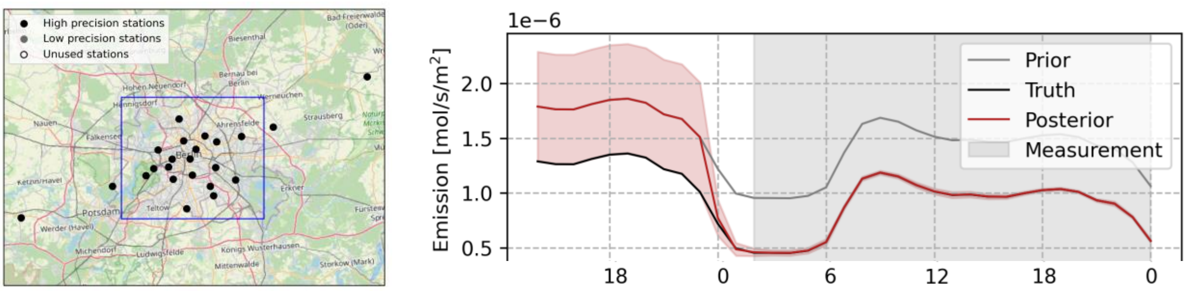

Fig 2: Using a sensor network in Berlin (left) within a Bayesian inversion enables the correct estimation of total CO2 emissions after a spin-up time (right), if the prior structure is known.

2023). While this prototypical setup shows that the inversion is technically successful, the results are still highly dependent on the chosen inversion setup, such as the structure of the 'prior' information and the desired resolution of emission estimation. In the next step, we will adjust the inversion settings to be realistic. Then, a quantitative analysis, including the examination of co-emitted substances, can take place.

WP3: AI driven plume detection and flux estimation of CO2 point sources from satellite data

This work package was carried out under our partner project (bd1231). Therefore, no ressources were used here.

WP4: Flexpart-ERA5 Simulation: Attributing CO2 variations observed in satellite records

Using Flexpart-ERA5, we were able to analyse the fire season 2019/2020 in Australia using – for the first time- TCCON measurements in Wollongong and Darwin. We calculated footprints using Flexpart and analysed the fire emissions quantitatively in an inversion. We have achieved considerable methodological improvement by analysing the optimal size of state vector and by including a coupling of CO and CO2 in the inversion framework. With these improvements, we were able to estimate fire emissions based on the TCCON stations, which are in agreement with fire databases provided by GFAS, but deviate substantially from GFED (see Fig. 3). We are confident that our methods are robust and now seek to utilize this framework in the future exploiting even more measurement data and including am optimization of biogenic fluxes alongside fire fluxes.

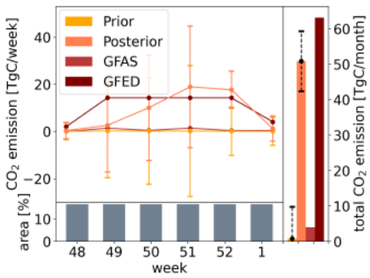

Fig 3: Comparison of posterior and prior fire CO2 emissions to GFED and GFAS for coupled inversion in Southeast Australia. Taken from: Dillerup, 2023.

Additional remarks:

1. We have additionally transferred the model GRAMM/GRAL to Levante to test its performance on a super computer. We were able to conduct model simulations (Fig. 4) and optimize the set-up with respect to storage usage and node hours. As the usage of a supercomputer enables us to conduct much faster simulations, we will request resources for running GRAMM/GRAL in the next request period.

2. Note that within our project Bachelor, Master and PhD students worked on Levante to finish their thesis. While this has not led to a publication between 06/2023 to 03/2024 yet, they were able to make substantial progress with and in some cases finish their theses.

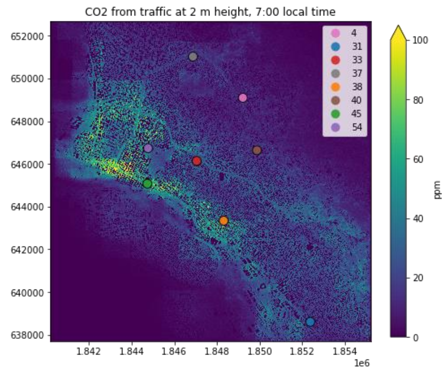

Fig 4: The simulation of CO2 with GRAMM/GRAL can be conducted efficiently. This enables comparison with observation data (colourful dots). Comparison of posterior and prior fire

References:

Maiwald, R. Lüken-Winkels, C. : [Code] ATMO-IUP-UHEI/BayesInverse: V.1.1 release of BayesInverse (v.1.1). Zenodo. https://doi.org/10.5281/zenodo.8354902, 2023

Dillerup, Ines, Master thesis: Inversion-based Wildfire CO and CO2 Emission Estimates for the Australian Extreme Fire Season 2019/2020 using FLEXPART, 2022