Project: **bm1400**
Project title: **Integriertes Treibhausgase-Monitoringsystem für Deutschland (ITMS)**
Principal investigator: **Dr. habil. Christoph Gerbig**
Reporting period: **2024-11-01 to 2025-10-31**

Achievements during the reporting period

Computation time and disc space: The ITMS's involvement with the DKRZ project bm1400 has focused on modules M and Q&S. The following achievements with the HLRE platform during the previous allocation are thus reported as follows:

Module M:

1. CSR + STILT (0.25 x 0.25 degrees):
   Biogenic CO2 flux estimates are calculated using CSR with STILT (0.25 x 0.25 degrees) over the domain of Europe for 2006-2024. The spatial distributions of 2024 flux estimates show that the European domain is a weaker sink of CO2 than suggested by the prior biosphere model VPRM (see Figure 1). The inversion estimates are guided by the atmospheric observations collected from 59 in situ atmospheric stations (ICOS and non-ICOS) distributed all over Europe.
   In addition to the CO2 and CH4 inversions, the CSR system has also been used to perform a joint CH4 and Radon (Rn) inversion for 2021-2023. This dual-tracer inversion exploits the fact that the transport model error between these two gases is correlated. Figure 2 illustrates how the additional Rn information affects the CH4 flux estimates in Germany.

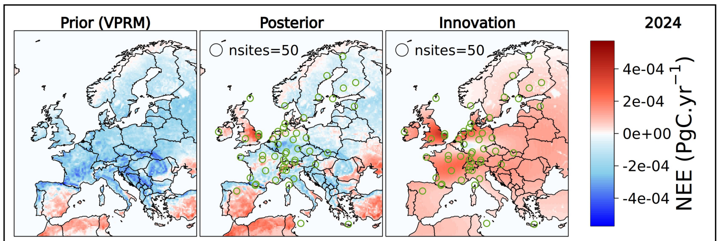

Figure 1. *Prior CO2 fluxes calculated with the biosphere model VPRM (left), posterior fluxes estimated using CSR (middle), Innovation of fluxes (posterior – prior, right).*

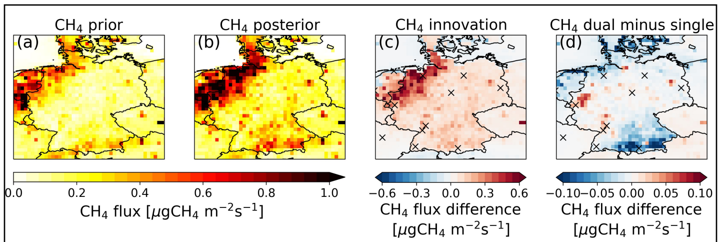

Figure 2. *Results of the CH4-Rn inversion: Shown are the CH4 prior (a), posterior (b), and posterior-prior difference (c) of the dual-tracer inversion. The difference between the CH4 flux results of the dual-tracer and the single-tracer CH4-only inversion are shown in* (d). *The locations of the observation sites are marked with black crosses.*

2. ICON-ART - CTDAS (R3B08, ~6.5 km resolution):
   After the previously successful synthetic experiment of inversions using ICON-ART–CTDAS with pseudo observations, we attempted to assimilate actual satellite XCH4 data from the TROPOMI WFMD product. Within Europe, a total of 944,845 satellite observations over the course of 30 days were assimilated, aiming to provide CH4 emission estimates for June 2018 (Figure 3). In order to work with the EnKF-based inversion system CTDAS, a configuration of ensemble simulations carrying 100 tracers needed to be carried out. This required significant resources from Levante for both computational and storage. However, with the initial attempt to assimilate real data, the result shows unrealistic posterior emission estimates, indicating an issue from the inversion setup to be resolved before proceeding to the originally planned 1 year long CH4 inversion estimates. Nevertheless, we have identified several shortcomings and are currently working on potential solutions to overcome them. The results have been much improved by incorporating optimization of the background fields, and reduction of transport error by frequent re-initializations. Instead of looking at a single assimilation cycle, it is expected that reasonable results can be finally achieved when multi-cycle inversions are carried out, thus converging the extreme scaling factors.

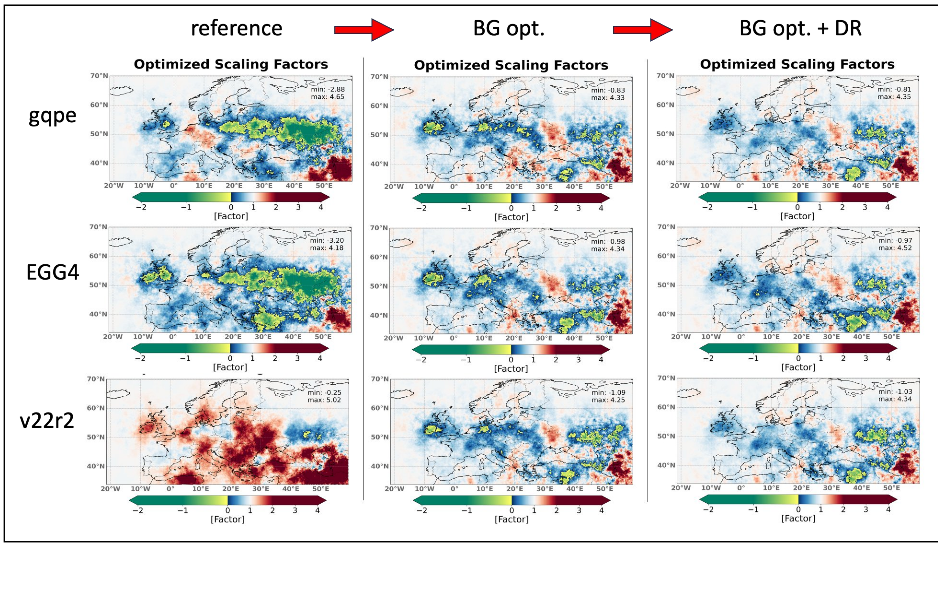

Figure 3. *Preliminary results of the CH_4 inversion with a single cycle using ICON-ART–CTDAS assimilating 10 days of satellite observations for June 2018 over Europe. Despite having passed the pseudo-truth experiment, we exhibit unrealistic result in the reference run (e.g. negative posterior fluxes). The result has been much improved by incorporating optimization of the background fields, and reduce transport error by frequent re-initializations.*

3. ICON-ART OH chemistry and lifetime:
A set of global ICON-ART forward simulations has been carried out in a lower resolution to test and compare the new super-simplified OH (SSOH) chemistry against the more sophisticated simplified OH chemistry and the much simpler lifetime approach. These show that the SSOH chemistry achieves the same computational performance as the lifetime approach and thus has a massive speed advantage compared to the simplified OH chemistry. At the same time, SSOH provides OH fields and methane depletion rates comparable to more complex simplified OH chemistry and much more sophisticated than the lifetime approach.
On top of that, a set of model transport tests (the so-called terminator toy chemistry) have been carried out to estimate intrinsic model transport error. The full analysis of the results is still in progress.
4. WRF-CHEM (1km resolution):
We have analysed the sensitivity studies of WRF-Chem runs. We showed that the choice of urban canopy and planetary boundary layer schemes has the largest impact on model performance, while station-specific characteristics also strongly influence the outcome. We have additionally identified the best overall configuration of physics schemes for urban areas, which we now use for follow-up studies, e.g. analysing aircraft camapign data over urban areas to quantify the emissions. Pilz et al. 2025: https://doi.org/10.1016/j.atmosres.2025.108435
5. Comparison of inversion results:
Module M produces inversion results from different groups and inversion systems. A centralized storage, comparison, and visualization of these results has been started on levante, using the fluxy tool and the corresponding data format (see Figure 4). The easily accessible comparison has proven highly valuable for the cooperation within the module.

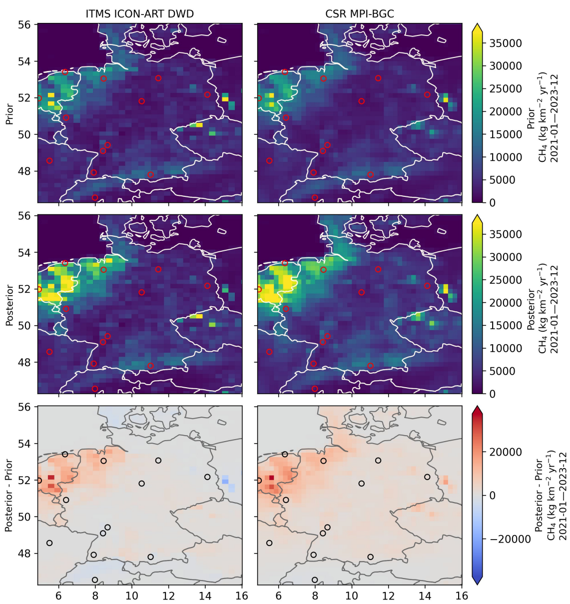

Figure 4. *Comparison of inverse model results for CH4 from MPI-BGC's CSR (left) and DWD's ICON-ART-based inversion (right) using DKRZ's jupyter hub showing the prior emissions (top), posterior (center row), and innovation (bottom) averaged over three years (2021-2023). This exemplified how different research groups within ITMS-M collect their results on levante and visualize the data using the fluxy tool.*

Module Q&S:
LandscapeDNDC (KIT IMK-IFU): In 2025 the modelling framework was transferred from the local HPCs at KIT Campus Alpin and Karlsruhe to Levante. This transfer included modifications and adaptations, leading to delays in the use of node hours in 2024 and the beginning of 2025. However, once completed we were able to quickly take advantage of the power of Levante, due to the effort spent in ensuring the flexibility of the modelling framework. The main result is that we have determined N2O emissions from agricultural soils at the district level, including a full uncertainty quantification, and shown that the uncertainty can be considerably reduced compared to the current methods used in the National Inventory Report (see Figure 5). The uncertainty quantification is crucial for both GHG reporting and for producing prior estimates for inversion modelling, but is by its nature computationally expensive. In particular, we use Bayesian techniques for assigning model parameter-set likelihoods and importance resampling of these parameter sets for inclusion in a Monte Carlo uncertainty analysis, both of which need significant computational power. CO2 exchange for German forests has been determined on a similar spatial, but so far without uncertainty quantification. Further developments include simulating the seasonal pattern of N2O emissions, which show good agreement with inversion modelling, and determining soil radon emissions for use in joint methane-radon inversion modelling.

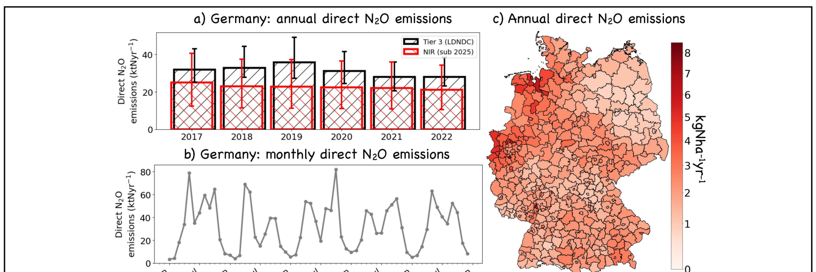

Figure 5. *LandscapeDNDC (LDNDC) estimates of N2O emissions from agricultural land for 2017 - 2022. a) Comparison of LDNDC results (black bars) with the current National inventory report (Submission 2025, red bars), including uncertainty quantification. b) Seasonal N2O emissions. c) Spatial disaggregation of N2O emissions at the Landkreis scale.*

<u>Additional benefits from Swift Object Storage (future S3 Storage):</u>

The additional benefits of the Swift Object storage space or the envisaged S3 storage have so far been used to submit deliverables generated for work packages within the modules (e.g., model output from LandscapeDNDC for use by Module M). With the transition to a future S3 system, we see important advancements. In ITMS, on its way towards an operational system, it is of utmost importance to document version changes in code but also in underlying datasets used to generate datasets in Module Q&S, which are then combined and used by Module M. Therefore, the SwiftStorage is a way to store and provide these data to ITMS-internal but also external partners. This is a significant advancement over the storage available only in the work directory.