RC2: 'Comment on egusphere-2025-4938', Anonymous Referee #2, 12 Dec 2025

The manuscript presents a dual state inversion framework developed at Yonsei University to estimate CO_2 and CH_4 emissions over Korea. The inversion is based on a coupling of DART and WRF-Chem, two widely used (and published) tools, so there is not a lot of technical novelty, but the setup itself is rather uncommon (at least in the GHG inversion field).

I guess the aim of publishing this in GMD is to have a published setup for referencing in future studies? This is totally fine, but then the authors need to do a little more than just presenting their coupling and one use case. They should clarify the interest (and drawbacks) of their dual-state setup, and justify the settings they used (uncertainties, correlations, resolution, choice of variables to be optimized, data selection, etc.). This should be demonstrated (e.g. through sensitivity experiments), not just stated. Currently the paper just shows the results of one single experiment, without really delving into what makes it a good experimental setup. That's a bit light. I also don't think that the comparison with the CAMS global GHG reanalysis is very insightful.

Overall though, what is written is well written, the topic is important and the setup is interesting, so the paper should eventually get published, once these comments have been addressed.

>> We thank the reviewer for this overall assessment. As suggested by the reviewer, we revised our GMD model-description paper to demonstrate the value of the configuration beyond a single use case. The goal of this study is to provide a fully documented, reproducible WRF-Chem/DART dual-state, dual-species (CO_2/CH_4) regional inversion workflow, and to demonstrate its behavior using both real-data experiments and a controlled OSSE, so that the community can apply and extend the system to other regions and observing systems. Accordingly, in the revised manuscript we demonstrated these issues by (1) clearly articulating what is enabled by our specific dual-state, dual-species configuration, (2) transparently documenting and justifying the numerical and methodological settings (uncertainties, correlations/localization, resolution, optimized variables, and data selection), and (3) providing targeted demonstrations (e.g., OSSE/sensitivity tests) that the setup behaves as intended. To address these concerns, we substantially revised the manuscript as follows:

1. Clarified the interest and architecture of the current model system configuration.
   We now explicitly provide detailed descriptions of our DA configuration with the augmented state vector and the explanation of the dual-state mechanism: meteorology and tracer concentrations are updated directly, while emissions/flux parameters are updated through ensemble-estimated concentration–flux cross-covariances. (Section 2.2). We also added a concise discussion of key trade-offs such as computational cost to other kinds of inversion systems.

2. Made the configuration choices traceable and reproducible, and justified "why these settings."
   We expanded the technical description (Section 2.2) with a step-by-step cycling workflow

and a compact configuration summary covering: optimized variables, cycling window, localization/inflation, observation types and selection, and prior uncertainty magnitudes. We also added input harmonization details (regridding and temporal disaggregation) at each data introduction point (Sections 4 and 5.1–5.4). In addition, we clarified the rationale for key uncertainty settings: 5% IC/BC perturbations as a pragmatic spread-maintenance choice for EGG4-based inflow fields, and 30% prior emission uncertainty tied to the empirically observed inter-inventory spread for South Korea (EDGAR/ODIAC/ROK-BTR), with explicit scope caveats and harmonization statements (anthropogenic CO_2 excluding LULUCF; consistent spatial aggregation and units).

3. Added controlled demonstrations and sensitivity-style tests to go beyond a single experiment. To provide quantitative evidence that the configuration is a sound experimental setup, we added a twin-style OSSE (Section 6) to test algorithmic consistency and flux recoverability under a known truth (imposed prescription of sector-specific emissions), reporting uncertainty reductions. Our OSSE-style denser-network scenario illustrates how increased information content leads to stronger and more spatially localized uncertainty reduction within the same framework, thereby effectively recovering regional emission signals and separating observing-system limitations from methodological limitations.

4. Reframed the CAMS/EGG4 comparison to increase relevance.
   We clarify that EGG4 is used as the prescribed IC/BC product; discussion of documented EGG4 biases is included only as diagnostic context for boundary-condition uncertainty that helps interpret posterior behavior and limitations (especially for CH_4), rather than as a validation target.

5. Better Documentation of parameterization and configurations incorporated in the system for complex terrain.
   Our system is based on established community tools, enabling the wider research community to apply it with different options. In addition, because near-surface transport is critical for high-resolution inversions over complex terrain, we note that our WRF configuration incorporated surface-layer/canopy-related options (e.g., roughness sublayer and canopy-height adjustments, Section 2.1).

Overall, these revisions are intended to make the manuscript a useful, citable reference for future studies: a fully specified and reproducible coupled WRF-Chem/DART dual-state, dual-species regional inversion workflow, accompanied by clear design rationale, documented configuration choices, and targeted controlled tests that demonstrate stability/consistency while transparently stating limitations and robustness considerations. We appreciate for your constructive comments.

Specific comments:

- The method description isn't sufficiently clear around what exactly is solved for by the data assimilation system. It seems to adjust the emissions (so it's an inversion?), but, according to Section 2.1, it adjusts meteorological and tracer fields (so it's an atmospheric state data assimilation?). Having some mathematical description of what happens (i.e. some equations) would help a lot. I assume it's an inversion, because emission adjustments are presented. I wonder if the tracer fields are directly modified by the assimilation as well?

>> As suggested by the reviewer, we substantially expanded the methodology description. In the revised manuscript (Section 2.2), we explicitly define the system as a joint state and parameter estimation framework using state augmentation. We also document the coupled WRF-Chem/DART cycling workflow step-by-step and summarize key configuration settings used in this study for reproducibility. Finally, we include more standard DART/EAKF references and documentation for readers who want additional algorithmic details. We also clarify that the 3-D tracer fields are directly modified by the analysis step. We now clearly articulate that:

(1) Atmospheric State (Direct Update): Meteorological variables and the 3-D CO_2/CH_4 concentration fields are included in the state vector (x_{met}, x_{chem}) and are directly updated at each analysis time using observations (i.e., standard sequential atmospheric state data assimilation). This joint update helps to maintain dynamical and transport–concentration consistency throughout cycling.

(2) Surface Fluxes (Indirect Update): Anthropogenic emission fluxes (x_{flux}) are included as unobserved parameters in the augmented state. They are updated indirectly through flow-dependent ensemble cross-covariances between the flux parameters and concentration innovations.

(3) A quantitative check of the data assimilation. We added a targeted OSSE to the revised manuscript, using an expanded 50-site synthetic surface network to test whether the framework can recover the intentionally imposed "missing power-industry" emission signal (a highly heterogeneous, point-source-dominated target) and to diagnose filter stability/consistency (including uncertainty reduction and innovation behavior). All OSSE configuration details and results are documented in Section 6 of the revised manuscript and Supplement for reproducibility. We emphasize that this OSSE is included to demonstrate algorithmic consistency and stability under controlled conditions; real-world performance remains influenced by transport errors, boundary-condition biases, and representativeness errors, which we discuss explicitly. The main focus of the manuscript remains the real-data demonstration.

To address the reviewer's request for explicit equations, we have added the concise mathematical description to Section 2.2 with proper references, including the definition of the augmented state vector ($x = [x_{met}, x_{chem}, x_{flux}]^T$) and the EAKF update equations that show how tracer-state updates occur directly while flux updates arise via ensemble-estimated cross-covariances (with covariance localization).

- The dual-tracer, dual-state setup is rather uncommon: what benefit does it provide upon a more classical inversion, solving only for emissions? What are the costs? This should be demonstrated, not just stated (i.e. through sensitivity experiments, at least). Even for more classical aspects (choices of uncertainties, correlations, data filtering, treatment of the boundary condition), at least some idea of what are the most impactful settings (within that particular inversion framework) should be provided. >> As suggested by the reviewer, we revised the manuscript to address this point quantitatively, consistent with the scope of a GMD model description paper.

1. Rationale and benefits of dual-state setup:

While emission-only inversions are computationally cheaper, we chose a coupled Eulerian framework to address the critical issue of transport error aliasing. By assimilating meteorological observations alongside tracers, we constrain the meteorological fields during the cycling window, reducing the likelihood that persistent transport biases are spuriously mapped onto flux corrections. In addition, the direct analysis update of 3-D tracer fields provides a necessary "state reset" at each cycle. This reduces the accumulation of background tracer errors in the cycling EAKF system, thereby limiting systematic over-adjustment of flux parameters across successive cycles in a sequential (cycling) inversion setting. The framework also yields a unified, dynamically consistent analysis of meteorology, tracer concentrations, and fluxes, which is essential for diagnosing transport-driven anomalies in complex terrain. Furthermore, the choice of a dual-tracer configuration reflects the primacy of CO_2 and CH_4 as the two most policy-relevant anthropogenic greenhouse gases in terms of their emissions and climate relevance, and they dominate national-scale mitigation and verification priorities. This setup allows the same regional DA and transport framework to be applied consistently to both primary target species within a unified workflow; however, we emphasize that we do not apply cross-species covariances and the two tracers are updated independently under the same constrained transport environment.

2. Costs and trade-offs:

Running a full ensemble of online WRF-Chem forecasts is significantly more expensive than offline transport-driven inversions. Moreover, the dual-state approach requires careful tuning of localization and inflation to manage sampling errors and maintain filter stability, making the setup more complex

than simple flux-scaling methods. We therefore document these controls explicitly to support reproducibility and clarify the primary tuning knobs for users.

3. Quantitative demonstration with a controlled twin-experiment (OSSE) and targeted sensitivities

To provide a controlled quantitative check, we added a twin-style OSSE (Section 6) showing that the system can recover a known truth (e.g., a prescribed power-sector emission perturbation), with associated uncertainty reduction and ensemble-consistency diagnostics. This OSSE also tests whether the chosen localization and error statistics propagate information from concentration innovations to flux parameters in a physically consistent manner. While a full emissions-only versus dual-state intercomparison across multiple cases would be a valuable follow-on, it is beyond the scope of this model-description paper.

4. Most impactful settings

We now explicitly document the controls that most strongly influence the posterior flux estimates within this framework, including localization (to filter spurious long-range correlations in the augmented state), the balance between prior spread and observation error (which determines the effective magnitude or "stiffness" of flux updates), and inflation (critical for preventing ensemble collapse in a cycling system). We also document the treatment of initial/lateral boundary conditions and the QC/filtering procedures, which strongly influence baseline gradients and the stability of cycling updates in a regional domain.

We believe this balanced discussion, acknowledging both the transport advantages and the computational costs, provides the transparency required for a GMD model description paper and responds to the request to indicate which settings are most impactful within this specific inversion framework.

- I think there is some confusion between high resolution transport and high resolution inversion. At line 369, you claim that: "the 0.75° x 0.75° resolution of EGG4 is not enough to resolve the sharp urban-industrial emission heterogeneity and fine scale sources and sinks across Korea. They motivate the use of high resolution regional inversion". It's quite obvious that fine scale processes will be better represented in a higher resolution model. But that doesn't mean that you "resolve" (as in, robustly constrain) the emissions at that resolution. You have three observation points, distant from each other by a few hundreds of kms, so you can't resolve emissions pattern at much finer scale. Finer-scale components of the posterior are mainly just carried forward from the prior. So at line 375, the statement that "Local increments of anthropogenic CO_2 and CH_4 emissions (...) are evident" is not really true: the increments appear local only in absolute magnitude. If they were shown as proportion to the prior uncertainties, they would appear as smooth, wide scale patterns. This is in fact very visible in Figure 10.

>> As suggested by the reviewer, we revised our manuscript to address this point properly, consistent with the scope of a GMD model description paper.

1. Clarification of "resolution" vs. "constraint."

We acknowledge that, with the current sparse network (three sites), the system primarily constrains broad, regional-scale modes of the flux field rather than independently resolving grid-scale emissions. We therefore revised the Results/Discussion text to remove wording that could be interpreted as "resolving" fine-scale sources at 9 km under the present observational coverage. We clarify that the motivation for the 9-km configuration is to reduce transport representation errors (e.g., complex topography, coastal circulations, and urban heterogeneity) that are critical for linking observations to regional fluxes, while the effective spatial scale of posterior flux constraint is set by network information content. Accordingly, at 9 km the posterior should be interpreted as a transport-consistent flux field whose independently constrained degrees of freedom are coarser than the grid spacing under the present network.

2. Reinterpretation of local increments

We agree that the term "local increments" in the original text could be misleading. We revised the phrasing to describe the posterior as "spatially varying adjustments within the localization-supported influence region," rather than evidence of independently resolved grid-scale corrections. Consistent with the reviewer's point (visible in Fig. 10; renumbered as Fig. 8 in the revised manuscript), the smoothness of posterior adjustments is an expected outcome of covariance localization and limited information content: with sparse observations, the posterior retains much of the prior's fine-scale spatial structure and mainly adjusts the large-scale modes that are observable given the network geometry and the imposed covariance and localization. We also delineate that apparent localization in absolute increments should not be interpreted as grid-scale resolvability when assessed relative to prior uncertainty or uncertainty reduction. In addition, the map shown is time-aggregated (period mean), so short-lived, flow-dependent increment patterns are smoothed and the figure primarily reflects robust, low-frequency adjustments supported by the available information content. We also clarify that the present application targets regional/national-scale constraints under the current network, rather than city-scale attribution as implied by the title.

3. Capability under denser coverage (controlled demonstration).

To separate observing-system limitations from methodological limitations, we added a controlled OSSE (Section 6) with a substantially denser synthetic surface network. Under this increased information content, the same framework yields stronger and more spatially localized posterior constraints and uncertainty reduction compared to the real-data three-site configuration. We present this OSSE as a capability demonstration under controlled conditions, without implying that the real-data three-site configuration achieves 9-km flux "resolution.

- The comparison with the surface concentrations in EGG4 ... just shows that EGG4 had a lower resolution, nothing more (so something that was known beforehand). In particular, it says nothing about the emissions, which is not a variable that EGG4 solves for, but which are your real target. Besides this comparison, the presentation of the results focuses mainly on the emissions, except for Figure 6 which shows the uncertainty reduction in the concentration space. I am however wondering how much the direct adjustment of the tracers (if it is done) compares with the adjustment of the emissions, and with that of the boundary condition, in contributing to improving the fit to observations. And does it make sense to adjust all of them? This needs to be better presented and justified.

>> As suggested by the reviewer, we clarified in the revised manuscript that CAMS EGG4 is used primarily as the prescribed IC/BC product. This revision addresses the reviewer's concern by clarifying that the EGG4 is used as the prescribed IC/BC forcing and by explicitly presenting the complementary roles of state and flux updates under prescribed boundary forcing. For better readability, we moved the corresponding figure(s) to the Supplement and revised the surrounding text accordingly.

1. Role of EGG4: not an emission comparison and a validation target

   In this study, CAMS EGG4 provides CO_2/CH_4 initial and lateral boundary mole fractions for the WRF-Chem/DART cycling simulations (with small ensemble perturbations to maintain boundary spread). We have revised the text to clearly state that the comparison with EGG4 concentrations is not intended as an emissions evaluation. Instead, it is used only to provide context on the limitations of coarse-resolution background forcing and to motivate why high-resolution regional transport is needed to represent sharp gradients and mesoscale flow–terrain effects over Korea.

2. Drivers of improved fit to concentration observations in our configuration

   We revised Section 2.2 and Results section to make the roles of each component explicit. In our cycling EAKF configuration, meteorological variables and 3-D tracer mixing ratios are updated directly with their respective observations at analysis times, while emissions/flux parameters are updated indirectly through flow-dependent ensemble cross-covariances between flux parameters and tracer innovations (state augmentation). Consequently, the immediate improvement in the analysis-time fit is driven primarily by the direct state update, whereas emission updates contribute to the persistence of improvements across cycles by correcting the emission input for subsequent forecasts (e.g., reduced recurring innovations and improved short-term forecasts). We emphasize in the revised text that updating both state and flux is therefore meaningful and complementary in a cycling inversion framework.

3. Why boundary conditions are not competing "controls" in this configuration.

   Lateral boundary mole fractions are prescribed from CAMS EGG4 and are not treated as state vector (control variables) in the analysis. The post-analysis boundary procedure (update_wrf_bc) is applied solely to maintain numerical consistency near the boundary relaxation zone and avoid discontinuities, rather than to tune external inflow. Therefore, the system does not involve a trade-off between boundary tuning and emission estimation; boundaries are prescribed, while within-domain state and flux updates operate as described above. We note, however, that residual errors in prescribed boundary forcing can still project partially onto within-domain concentrations and inferred flux adjustments; we therefore interpret boundary-related diagnostics separately from within-domain emission increments.