Author response to reviewer comments

Anonymous Reviewer #2

The authors have now included much more detail about their technical methodology to estimate emissions from dispersed sources. I have some specific questions about this new section, but otherwise the manuscript is much improved.

We thank the reviewer for their helpful comments on the revised manuscript. We addressed the reviewer comments and revised the manuscript in the SI section where the methodology is described. Our point by point responses to all comments are below in blue.

1. Section S1. Equations in SI - make sure you are using consistent notation for vectors vs matrices. H is a matrix in Eq S1 and s is a vector, correct? Please use consistent notation

Thank you for identifying this error. We have corrected the equations in the SI (section S1) to use consistent notation.

2. Section S1. "The inclusion of fixed discrete sources in the inverse model makes this a constrained regularized optimization rather than Bayesian inference, and so we report only the optimal solution and do not assign probabilistic confidence intervals. It is important to note that this is non-Bayesian to prevent overinterpretation of a "posterior" estimate, which would be invalid due to data re-use." I'm not sure I agree with the first sentence as written. What makes this non-Bayesian is the fact that you are applying regularization parameters and hard constraints in your optimization protocol, not because you have discrete point sources as a state element in the equation. For the second sentence, as written this is confusing. If you have truly separated discrete elements from dispersed elements, and fixed the discrete variable, I don't understand how data would be "re-used" if you were to apply a bayesian method, at least in a way different than a Tikhonov formulation. Please clarify.

We thank the reviewer for this clarification and agree that the original wording was imprecise. We have clarified the text accordingly in section S1.

First, we agree that the inclusion of discrete point sources as state elements does not, by itself, render an inverse problem non-Bayesian. The non-Bayesian nature of our approach arises from the way the diffuse inversion is formulated and solved: namely, as a constrained, regularized optimization with a fixed regularization parameter and hard constraints (non-negativity and a mass constraint), rather than as a probabilistic inference with explicitly defined priors, likelihoods, and uncertainty propagation.

Second, we appreciate the opportunity to clarify our use of the term "data re-use." In our framework, discrete source emissions are first estimated using a divergence-integral (DI) method applied to a subset of the MethaneAIR XCH_4 observations. These discrete emission rates are then fixed and treated as known quantities in the subsequent optimization for dispersed emissions. The dispersed emissions are inferred using an objective function that is evaluated against the full XCH_4 observation set, which may include observations that were previously used to estimate the discrete sources.

As a result, the same observations can influence both the discrete-source estimates and the dispersed-source solution, without explicit propagation of uncertainty from the discrete-source step into the dispersed inversion. A fully Bayesian treatment would require either (i) joint inference of discrete and dispersed emissions within a single probabilistic framework, or (ii) propagation of uncertainty from the discrete-source estimates into the dispersed inversion. Because neither is done here, interpreting the dispersed solution as a Bayesian posterior would be incomplete. For this reason, we deliberately adopt a non-Bayesian framing and report only the deterministic optimal solution of the constrained optimization, rather than probabilistic confidence intervals or posterior distributions. We have revised section S1to reflect this clarification and to remove the implication that discrete sources themselves make the problem non-Bayesian, as follows:

Section S1, p. 3: *"The same observations can influence both the discrete-source estimates and the dispersed-source solution, without explicit propagation of uncertainty from the discrete-source step into the dispersed inversion. A fully Bayesian treatment would require either (i) joint inference of discrete and dispersed emissions within a single probabilistic framework, or (ii) propagation of uncertainty from the discrete-source estimates into the dispersed inversion. Because neither is done here, interpreting the dispersed solution as a Bayesian posterior would be incomplete. Therefore, we deliberately adopt a non-Bayesian framing and report only the deterministic optimal solution of the constrained optimization, rather than probabilistic confidence intervals or posterior distributions."*

3. Section S1. I have a question regarding lingering concentrations from discrete elements: "Discrete sources are fixed in the area source inversion, fixing emissions in a 0.01° x 0.01° area, which approximates the effective representative area of the DI." As I understand, the DI approach assumes that for a discrete source, there is downwind concentration that hits the boundary of a square tile. The implication is that there is likely additional concentration that extends beyond the 600 m tile, and potentially beyond a 0.01 degree grid cell that encloses that tile if the plume is sufficiently large. By not segmenting, accounting, and

attributing those concentration enhancements to the discrete sources from which they originate, those enhancements now get lumped/used in the inversion for s_dispersed. Do you account for that potential source of bias and how? Or clarify how this does not incur potential bias in the result for s_dispersed.

We thank the reviewer for bringing to light this important clarification. In our framework, discrete sources are incorporated as fixed state elements in the inverse problem by fixing the emission rate of the grid cell containing the detected source. Consequently, downwind concentration residuals associated with discrete sources are, in principle, available to be fit by the diffuse emission field. This design choice was intentional and reflects a prioritization of accuracy of total emissions over the spatial distribution of the dispersed emission field. Our paper is entirely focused on total emissions from the individual regions.

If we attempted to segment the observable downwind enhancements due to the discrete sources, we would inevitably 1) underestimate the total enhancement from the discrete source where those enhancements fall below detectability (i.e., under-estimate the extent of the plume due to observation noise), and/or 2) overestimate the total enhancement by lumping other sources into the segmented downwind enhancement. By fixing the discrete source to the DI estimate, we allow the Jacobian and hard mass constraint to close the total methane emissions budget.

The diffuse emission inversion is formulated to explain the observed enhancement field subject to non-negativity, smoothness regularization, and a hard mass constraint. Under these constraints, any residual signal downwind of a fixed discrete source is preferentially distributed smoothly over the surrounding area rather than producing localized artifacts. As a result, plumes from discrete sources are effectively absorbed into the local diffuse field with only small downwind effects and without introducing spurious secondary discrete sources.

We acknowledge that this approach may attribute some fraction of discrete-source plume tails to the diffuse component, and we have clarified this explicitly in the revised SI. However, this attribution does not affect the basin-integrated emission total, which is constrained by the hard mass constraint.

Section S1, p. 3: *"We acknowledge that this approach may attribute some fraction of discrete-source plume tails to the diffuse component, but this does not affect the basin-integrated emission total, which is constrained by the hard mass constraint."*

4. Section S1. "The solution is initialized to a flat field that satisfies the mass constraint. Subsequent proposals are constrained to be non-negative and satisfy the mass constraint. The two constraints regularize the solution to prevent overfitting." Reducing overfitting in a Tikhonov scheme is also accomplished by the regularization parameter lambda. I don't see anything in the SI of how you choose that parameter, or is that parameter chosen as a result of the other constraints? Please clarify especially with respect to these other constraints.

The constraints and the Tikhonov term serve complementary roles: non-negativity enforces physical feasibility; the hard mass constraint enforces domain-scale consistency; and λ controls spatial roughness and suppresses fitting of retrieval/transport noise at small scales. A value of $\lambda=0.5$ was selected using an L-curve criterion computed over a set of representative scenes. We have added this information in the SI:

Section S1, p. 3: *"The non-negativity and mass-balance constraint are complementary to the Tikhonov term such that non-negativity enforces physical feasibility, the hard mass constraint enforces domain-scale consistency, and λ controls spatial roughness and suppresses fitting of retrieval/transport noise at small scales. A value of λ=0.5 was selected using an L-curve criterion computed over a set of representative scenes."*