Response to Reviewer 2

We would like to sincerely thank Reviewer 2 for their thorough evaluation of our manuscript and for the constructive comments and suggestions provided. We deeply appreciate the time and effort devoted to reviewing our work. The feedback has been invaluable and has contributed significantly to improving the quality and clarity of the manuscript. Below, we address each of the comments in detail.

Major Comments

- **Reviewer Comment:** ***Application to satellite data assimilation: The authors suggest that their approach is intended for use in satellite data assimilation. However, they do not present any data assimilation experiments. Such experiments are important, as there may be problems when using this approach in such applications. In data assimilation, the difference between observed satellite radiances and those simulated from model state variables (via RTTOV) is used to update the relevant model state variables. If LASSO induces sparsity by zeroing out many regression parameters, it removes the sensitivity of radiances to certain model variables or layers. As a result, assimilating those radiances may influence fewer aspects of the model state in terms of both variable type and vertical level. This could be undesirable. Therefore, data assimilation experiments are necessary to assess how the induced sparsity affects the assimilation of radiances.***

  Authors Response: We thank the reviewer for this insightful and important comment, which touches on a key consideration in the practical application of our method. We fully agree that the use of sparsity-inducing models such as ours in the context of satellite data assimilation requires careful evaluation, especially regarding the sensitivity of simulated radiances to the underlying model state variables.

  As correctly pointed out, LASSO-based regularization, by setting many regression coefficients to zero, may reduce the sensitivity of the forward model to certain variables or atmospheric layers. This could, in turn, limit the ability of the data assimilation system to propagate observational information through the model state, both vertically and across variable types. Therefore, conducting assimilation experiments is indeed crucial to assess how this sparsity impacts the effectiveness of radiance assimilation.

To address this concern and strengthen the manuscript, we will incorporate a new section in the revised version where we evaluate the performance of Fast-RT as a forward operator. While a full data assimilation experiment is beyond the scope of the present study, this first evaluation step aims to provide a diagnostic of the model's realism in simulating satellite radiances.

In particular, we will compare the brightness temperatures (BTs) produced by Fast-RT to those obtained from high-fidelity simulations from LBLRTM. The key criterion we propose is that the absolute difference in BT must be lower than the instrument's noise level: the Noise Equivalent Delta Temperature (NEdT) for the thermal emissive bands (M12–M16), and the Noise Equivalent Delta Radiance (NEdR) for the solar reflective bands (M7–M11). It is clear that any radiance below the instrument noise cannot be detected by it, so the assimilation of these satellite data is sufficient as long as the models, whether Fast-RT or line-by-line, are as accurate as what the instrument can measure.

We suggest that the percentage of atmospheric profiles for which this condition is satisfied constitutes a meaningful and practical metric to evaluate the quality of the forward model. A high proportion of profiles with errors below these thresholds indicates that the model error is smaller than the sensor noise and, therefore, that the simulated radiances are sufficiently accurate for use in satellite retrievals and potentially for data assimilation. This criterion provides a quantitative benchmark aligned with the capabilities of the instrument and the intended application.

We acknowledge that this evaluation does not replace the need for actual data assimilation experiments, which will be an essential next step in future work. Nevertheless, we believe that the proposed analysis offers a relevant and informative proxy for assessing Fast-RT's suitability in assimilation contexts and complements the objectives of reducing computational cost in operational or research-oriented inverse problems.

We will clearly state these points in the revised manuscript, along with the corresponding validation with respect to the VIIRS instrument noise level, and include the results of this performance assessment as a foundation for further developments.

- **Reviewer Comment:** ***Further explanation and interpretation of results: In Sections 5.3 and 5.4, the authors provide a numerically detailed discussion of the approximation errors introduced by LASSO. However, it would be beneficial to provide a theoretical interpretation of these results. Specifically, is there a link between the approximation error and the number of non-zero parameters and the characteristics of individual channels? Do the authors believe that the observed variations in performance are largely due to random effects?***

  Authors Response: We thank the reviewer for this insightful comment, which deepens the understanding of our model's behavior and highlights an important area for further analysis. We agree that providing a theoretical interpretation of the approximation errors induced by LASSO regularization is essential, especially in relation to the sparsity level and the specific characteristics of each spectral channel.

In particular, and in connection with our first reviewer comment on evaluating model errors relative to instrument noise, we will extend the revised manuscript to include a comprehensive theoretical discussion focused on how the inclusion or exclusion of gases and predictors affects the approximation error. This discussion will clarify how the error depends on the number of non-zero regression parameters and the modeling choices made. We emphasize that the observed differences in error between RTTOV and our Fast-RT model are largely attributable to the tuning of the tolerance parameters ϵ_1 and ϵ_2. To demonstrate this, we will include a table showing how reducing these tolerance thresholds results in lower approximation errors, highlighting the trade-off between achieving sparsity and maintaining accuracy.

Furthermore, for channels close to the visible spectrum (solar reflective bands), the larger errors observed with respect to LBLRTM are not primarily caused by the sparsity induced by LASSO, but rather by simplifications in our radiative transfer model—most notably, the omission of the solar radiation component. Addressing this limitation by explicitly incorporating solar radiation effects is part of our planned future work, which we expect will substantially improve the physical realism and accuracy of our model in these spectral regions.

By including this theoretical analysis and clarifying these aspects, we aim to provide a more complete understanding of the error behavior observed in our results and to set the stage for ongoing improvements.

- **Reviewer Comment:** ***Acronyms: There are lots of acronyms used in the paper. While some might be familiar to many readers, it would be helpful if the authors could provide the full name where they first appear. This applies to both the abstract and the main text.***

  Authors Response: We thank the reviewer for this helpful suggestion. We acknowledge that the excessive use of acronyms can hinder readability, especially for readers who may not be familiar with all terms. In the revised manuscript, we will ensure that all acronyms are fully spelled out with their corresponding definitions at their first appearance. This will improve the clarity and accessibility of the paper.

- **Reviewer Comment:** ***Formatting issue with citations: This issue appears in many places (e.g., lines 20-24, lines 32-35 and lines 54-57). For example, on line 54, it should be "... optical images (Hong and Kong, 2021) ...***

  Authors Response: We thank the reviewer for identifying these specific instances. We will carefully review the manuscript to correct the mentioned issues and ensure that citations and phrasing are accurate and consistent throughout the text.

Specific comments:

1. Line 1: This sentence is slightly misleading. In data assimilation, radiative transfer models map model state variables (e.g., temperature) onto the radiances measured by the satellite. It is the radiances that are assimilated, rather than the retrieved

temperature.
Response: The first sentence of the abstract has been revised to: The assimilation of satellite spectral sounder data ~~requires fast and accurate radiative transfer models for retrieving surface and atmospheric variables~~ **relies on fast and accurate radiative transfer models to simulate satellite radiances from surface and atmospheric state variables.**

2. Line 11: Move "(RT)" forward to be after "radiative transfer"
Done.

3. Line 11: Again, this sentence is a bit confusing. What the authors describe in the following two paragraphs is exactly what the reviewer expected!
Changes: In satellite data assimilation and remote sensing retrieval, as well as their applications in numerical weather prediction (NWP), the radiative transfer ~~equation (RT) is the principal model used to retrieve global atmospheric variables, such as temperature and trace gases concentrations, including water vapor, ozone, carbon dioxide, and other atmospheric constituents.~~ **(RT) equation is the forward model relating atmospheric state variables to satellite-observed top-of-atmosphere (TOA) radiances across different electromagnetic spectrum channels.**

4. Lines 39-40: Even for large centres where RTTOV is being used operationally, the proposed approach has benefits if it reduces computation costs while maintaining accuracy.
Response: We appreciate the reviewer's comment. Although RTTOV is used operationally in large centers, our approach offers computational savings while maintaining accuracy, benefiting both large centers and smaller agencies.

5. Line 64: Could the authors provide slightly more clarification at line 50, where it states that LASSO regression has been applied in the context of radiative transfer in Cardall et al. (2023).
Response: The input data used were not raw radiance values, but rather reflectance products and other variables derived from different Landsat spectral bands, including ratios and transformations relevant for chlorophyll-a and turbidity detection. While the approach does not model radiative transfer explicitly, it leverages empirical relationships between surface reflectance and in-water constituents.
Changes: LASSO regression was applied by Cardall et al. (2023) ~~to improve and estimate parameters in water quality monitoring models with optically complex properties~~ **to estimate water quality parameters such as clarity, temperature, and chlorophyll-a, based on correlations with in situ measurements and near-coincident Landsat spectral data, with a focus on model explainability**.

6. Section 1.1: The reviewer recommend reformatting this subsection to the last paragraph of Section 1, as there is no Section 1.2.
Done.

7. Line 74: Reference for the monochromatic radiative transfer equation (Equation 1).
Response: referenced to Weinreb et al. (1981).

8. Line 134: Could the authors provide an example of the predictors for a given instrument

and gas?
Response: Appendix 2 has been added to provide the RTTOV v13 predictors for the gases considered in this study.

9. Equation (12): The second case is confusing because it states that $d_1 = \bar{d}_1$. How is d_1 on the right-hand calculated?
   Response: If this case occurs, i.e., transmittance shows low variability with respect to atmospheric variables but is not close to 1, then $\bar{d}_1 = -\ln(\bar{\tau}_1)$, where $\bar{\tau}_1$ is the mean transmittance computed across all 83 profiles and all 6 view angles at level 1 of the discretized atmospheric model.

10. Line 232: Readers could benefit from some further discussion on the selection of the thresholds ϵ_1 and ϵ_2.
    Response: These statistical threshold tolerances should be close to zero. This clarification is included in the manuscript, and the numerical experiments show results for different values of these tolerances. Moreover, a corresponding analysis is carried out to assess the impact of varying these parameters.

11. Line 245: Why is a factor of 2 used?
    Response: This represents a relative tolerance that specifies how close the mean squared error (MSE) of the LASSO solution should be to that of the ordinary least squares solution. Since $mse(\lambda) > mse(0) > 0$, the condition can be rewritten as $\frac{mse(\lambda)-mse(0)}{mse(0)} < 1$. We then select the largest value of λ among the candidates that satisfies this inequality. In the revised version of the manuscript, the Bayesian Information Criterion is used as a model selection tool for the same purpose.

12. Line 261: The full name of VIIRS should be provided earlier in the text.
    Done. The full name of VIIRS has been added in line 62.

13. Line 267: What does "SRF" stand for? Does it stand for "Spectral Response Function"?
    Change: Spectral Response Function (SRF). This is clarified in the revised version of the manuscript.

Minor Comments

1. Line 135: "de number of predictor" → "the number of predictors"
   Done.

2. Caption of Table 9: "Maximun Relative Errors" → "Maximum Relative Errors"
   Done.

3. Line 172: "... predicted by the model (8)." → "... predicted by the model (Equation 8)."
   Done.

4. Line 207: "... considering M angles and N atmospheric profiles ..." → "... considering N angles and M atmospheric profiles ..."
   Done.

5. Line 264: “In this study, we use the VIIRS SRF J2 and can be downloaded from the following link: ...” → “In this study, we use the VIIRS SRF J2, which can be downloaded from the following link: ...”
   Done.