Reviews to gmd-2022-63: ICLASS 1.0: a variational Inverse modelling framework for the Chemistry Land-surface Atmosphere Soil Slab model: description, validation and application

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The manuscript *ICLASS 1.0: a variational Inverse modelling framework for the Chemistry Land-surface Atmosphere Soil Slab model: description, validation and application* presents a new model iCLASS, based on the CLASS model to optimize variables and parameters in a simple Land-Surface Atmosphere model. The work behind the manuscript is impressive and very useful for the community. It will allow to better understand what drives interactions between the atmosphere and land surface.

However, despite the quality of the underlying work, including a detailed documentation, the full development of an adjoint, proper tests, etc., the manuscript in its present form is not suitable for publication in GMD.

The structure of the manuscript does not allow the reader to fully understand what has been done, in what context, and with what strengths and limitations. The manuscript should be extensively re-written and re-submitted when improved.

Below are axes of improvements and suggestions to improve the manuscript.

1 Introduction and bibliography

The introduction is not well-balanced and lacks pieces of bibliography. The reader would expect an extensive "review" of what has been done in parameter estimation in land-atmosphere exchanges, and not only with simple models. For instance, there has been some work on parameter estimations with full-physics models, such as ORCHIDEE or JS-BACH. The advantages vs drawbacks of simple models such as CLASS, compared to full-physics models should be more thoroughly presented. The scientific "ecosystem" of the present study should be better presented. There is a full field of studies using data assimilation, machine learning, etc.

The balance between giving only hints or extensive details is also clumpsy. For instance, in paragraph p.2 l. 34-48, the authors start giving information on the model itself compared to other models, but without going to the details. What is an "extensive set of observations"? What observations are better used than other models?

2 Energy balance and conditions of applicability of CLASS

The CLASS model is a simplified model with all its benefits and drawbacks. In particular, what are the conditions of applicability of CLASS? The authors mention "golden days" several times in the text. What are these? How frequent are they? If there is only a few such days per year, the model is not really suitable for purpose...

About the energy balance and further assumptions, it is not fully clear what is the domain of applicability of such assumptions. In particular, the advection and entrainment in the model are extremely simplified. What values and variables are used to constrain the processes?

3 Section 3.1 and mathematical notations

Please make your mathematical notations consistent with the rest of the community.

- prior vector: $\mathbf{x}^{\mathrm{b}}$: The author should explicitly write it somewhere, with all its sub-components (bias, parameters, inputs, etc.)
- posterior vector: $\mathbf{x}^{\mathrm{a}}$
- full observation operator: $\mathcal{H}$
- adjoint sensitivities are usually noted as: δS^{*}_{win}

Overall, Section 3.1 is very hard to understand. It is not clear at all what is optimized or not. The section gives some general information about the inversion framework, but does not go to the necessary level of details about what exactly is in each mentioned vectors and operators. The dimension and content of all operators and matrices should be detailed.

The weights on observations or "regularization factors" are clumsy and not justified. If one observation is less worthy than another, then the uncertainty should just be scaled up, with no need for an extra complicated parameter.

Equation (6) is too implicit. The author should fully detail the "background" term, including what they optimize or not.

4 Uncertainties and OSSEs

Please provide extensive details on the uncertainties you specify for the inputs and parameters and some justification for the corresponding uncertainties. In particular, for parameters, the normal distributions are not necessary the most obvious choice. This should be justified and detailed.

The OSSEs are rather simple and do not fully allow to validate the model. More OSSEs should be made more systematically to show what is the influence of a given parameter in a given set-up. The author can perturb a parameter but not optimize it, etc. Besides, I may have missed the information, but I have the impression that the bias correction is not evaluated in the OSSEs. This should be added.

Regarding the posterior uncertainties, having truncated Normal distributions means that the minimum of the cost function is the node of the posterior distribution, which is not the mean or median, contrary to full normal distributions. Therefore, the authors should give further details on how the compute and analyze posterior distributions.

5 Details on the model

There is critical information missing about the CLASS and iCLASS models. Some of this information is given in the documentation of iCLASS, but not comprehensively. The reader cannot be expected to read the non-reviewed documentation to understand the article and how the adjoint is built.

In particular, there should be full details on the inputs and parameters of the CLASS models. What are the resolutions of each inputs? Where do they come from? Are they given by in-situ measurements? Meteorological forcing fields?

Similarly, what are the exact outputs of the model? How the output is compared to observations.

Finally, what is computed by the model? And what is given as inputs?

6 Superfluous sections and elements

The text is made hard to follow by numerous superfluous details.

For instance, section 4 is mainly made of a technical lecture on how to code an adjoint. This can be removed altogether.

7 Technical comments

1. p.1 l.9: replace "the core physics to model" by "the core physics to simulate"

2. p.3 l.63: The example is rather a negative feedback but not an obvious non-linearity. There are probably better examples.

3. p.3 l.66: "Analytical" is ill-chosen and refers to analytical inversions in the inversion framework. The adjoint is simply needed to compute explicitly and efficiently the gradient of the cost function, without relying on, e.g., finite-element estimations

4. Section 8: the validation of the adjoint using the gradient test and the test of the adjoint is really appreciated! The results of the test of the adjoint is generally reported as a N times the machine epsilon (10^16 in present machines)

5. p.15 eq.20: x_A is modified in the Monte Carlo.

6. p.15 eq.22: χ^2 formula is wrong for two reasons. First the chi-square diagnostics can be applied only with normal distributions. Truncated-Gaussians break the diagnostics; but for not so truncated Gaussians, it may still be valid.

   Second, the authors mixed two versions of the chi-square diagnostics: one from, e.g., from Michalak et al. 2005 (doi:10.1029/2005JD005970), the other from, e.g., Zupanski et al. 2006 (https://doi.org/10.1175/MWR3125.1). In one version the chi-square has a mean of n (nb obs) and in the other $n + m$ (nb obs + parameters). As written in eq.22, the expected mean is n, or the authors compute the other version, but should explain more clearly what is done.