Review : ICLASS 1.0: a variational inverse modelling framework for the Chemistry land-surface Atmosphere Soil Slab model: description, validation and application

1 GENERAL COMMENTS

The paper describes a novel variational inverse modelling framework for the one dimension Chemistry Land-surface Atmosphere Soil Slab model CLASS, which consists of a simplified land-surface model coupled to a model of atmospheric boundary layer. First, the paper shows a thorough presentation of the forward model and the associated inverse modelling framework, some illustrations of the adjoint coding and the description of error statistics. The adjoint model is validated technically using the tangent linear test and the adjoint test. Observation System Experiments show the strength of their approach to optimize land surface parameters. Eventually, the potential of ICLASS 1.0 at combining both large scale observations (e.g. CO2 mixing ratios) and local observations (e.g. CO2 flux) to constraint model parameters and to estimate bias in observations is demonstrated through an application for a grassland in the Netherlands.

This work can be expected to contribute significantly to improving our understanding of the terrestrial carbon cycle. Although briefly mentioned, the development of the inverse framework is a necessary step that presumingly aims to constrain the stomatal by combining observations of atmospheric mixing ratio and ecosystem fluxes of Carbonyl Sulfide at a specific location. The overall text is well written, and the authors very carefully present the framework, the experiments and discuss the results. The paper is within the scope of gmd and, I recommend its publication with minor amendments. Details of my comments will be found in the following.

2 SPECIFIC COMMENTS

Page 1, line 6: Replace "enables to estimate" by "enables the estimation of information".

Page 7, line 7: "free-tropospheric mixing ratios". I disagree, free tropospheric mixing ratios are not difficult to obtain by observations. There are numerous surface sites measuring greenhouse gases concentrations around the globe.

Page 1, line 19: Add an s after exchange.

Page 1, line 21; Strictly speaking, the second part of the sentence (the well known atm...) is false. The atmospheric boundary layer exists even though the daytime conditions are not sunny.

Page 2, line 30: Add after scalars (e.g. wind speed and temperature).

Page 2, line 30: For which time scale and horizontal resolution these assumptions are valid?

Page 2, line 35: Parenthesis within parenthesis. Use "for instance at Cabaw"..

Page 2, line 40: Here, you can mention the problems of equifinallity (Tang et al., 2008) and overfitting.

Page 2, line 42: Replace Inital by Initial.

Page 2, line 42: Replace e.g. by for instance.

Page 3, line 66: This is also illustrated in Ziehn et al. (2012) with the assimilation of atmospheric CO2 data in BETHY LSM.

Page 3, line 62: Above all, it is the iterative process that allows to find the local miminum of the cost function in case of linearity.

Page 3, line 65: The choice of using variational methods compared to other technics dealing with the non linearity (e.g. Particule filters) could be discussed here. The advantages of using an adjoint compared to a numerically computed gradient could be also added. For instance, the adjoint model is a tool that allows to obtain the sensitivities of model outputs to land surface parameters with more efficiency. The adjoint computation is also less expensive than computing the cost function gradient.

Page 4, scheme: By storage flux, do you mean tendency of the scalar (e.g dc/dt)?

Page 4, line 109: It would be worth defining what is Jarvis-Stewart approach compared to the a-gs module.

Page 4, line 120: I disagree. Within a Bayesian framework, inverse modelling does not necessarily involve any prior information.

Page 4, line 122: Delete others.

Page 5, line 125: Does it mean that the land surface model parameter are not optimised?

Page 5, line 138: The reference Chevallier et al., 2010 seems to me more appropriate than Chevallier et al. 2007 here. I would justify this assumption in an other sentence using .

Page 6, line 149: Add a coma after at this point.

Page 6, line 150: What is the point of adding some weights instead of inflating observational errors?

Page 6, line 156: Explain how si is distributed in Equation 5.

Page 6, line 165: Above all, this method is adapted for minimizing a non-linear cost function. Please specify the algorithm used. For instance, Raoult et al. 2016 used the L-BGFS-B algorithm as many others (see also Bastrikov et al., 2018; Kuppel et al 2014; Bacour et al., 2015).

Page 7, Figure 2: The figure should be more illustrative. As such, it does not help to understand the framework. At least, add the formula in the box. The iterative process should be also illustrated. See Figure 1 for instance of Thanwerdas et al., 2021.

Page 8, line 1: Specify why you optimize $Frac_H$ instead of ϵ_{eb}.

Page 8, line 229: It is well known that depending on prior parameters the optimisation can get stuck in a local minimum. Please cite a textbook here. See also Santaren et al., 2014 and Bastrikov et al., 2018.

Page 8, line 236: Cite Tarantola after the word approach.

Page 11, line 284: Specifify that the adjoint is computed for each iteration.

Page 13, line 362: Specify what are the arguments $checkpoint_init$ and $model$.

Page 13, line 362: The optimized emission factor can become negative as well..

Page 14, line 390, Remove one of the two "to".

Page 16, line 425: Specify that the chi 2 is only an indicator that can be misleading in particular when off diagonal terms are involved in the observation error matrix (Chevallier , 2007).

Page 17, line 470: Remove in after reads.

Page 18, line 483: "similar to Honnorat et al. , 2007". This is a standard test, please cite a textbook here or more references.

Page 18, line 490: It would be nice to show in a tabular the values of α and the associated results for the left and right sides of the equation.

Page 19, line 523: RevealS.

Page 19, line 527: OSSEs are classic to test the ability of the system to properly estimate model parameters..

Page 19, line 530, Start a new sentence after complexity and remove the coma after experiments.

Page 19, line 535: ""In the cost function..true parameters". The sentence need to be explained as prior information means to avoid the parameters taking unrealistic values.

Page 19, line 543: Add a coma after experiment.

Page 20, table 1: Previously, you wrote that you removed prior information. What does the prior column correspond to?

Page 21, line 566: as many iterations WERE needed.

Page 21, line 570: Add a coma after setup.

Page 23, line 596: Are shallow clouds represented in the forward model?

Page 23: Combine Figures 3 and 4 .

Page 26: Combine Figures 5 and 6.

Page 22, line 590: On Figure 5, the height and relative humidity show a less good fit to observations around noon. Is it because of the formation of shallow clouds?

Page 28, line 644: "The use .. model" Please explain this sentence (this is done through the use of OSSE such as e.g. Stinecipher et al., 2022).

Page 28, line 657: "It avoids..." Please explain.

Page 30, line 672: Give an example of small scale processes which are not represented.

Page 30, conclusion: You could also emphasize that the inverse framework serves at determining which observations are needed through the use of OSSEs.

3 Bibliography

Bastrikov, V., MacBean, N., Bacour, C., Santaren, D., Kuppel, S., and Peylin, P.: Land surface model parameter optimisation using in situ flux data: comparison of gradient-based versus random search algorithms (a case study using ORCHIDEE v1.9.5.2), Geosci. Model Dev., 11, 4739–4754, https://doi.org/10.5194/gmd-11-4739-2018, 2018.

Kuppel, S., Peylin, P., Maignan, F., Chevallier, F., Kiely, G., Montagnani, L., and Cescatti, A.: Model–data fusion across ecosystems: from multisite optimizations to global simulations, Geosci. Model Dev., 7, 2581–2597, https://doi.org/10.5194/gmd-7-2581-2014, 2014.

Chevallier, F., et al., 2010: CO2 surface fluxes at grid point scale estimated from a global 21-year reanalysis of atmospheric measurements. J. Geophys. Res., 115, D21307, doi:10.1029/2010JD013887

Frederic Chevallier. Impact of correlated observation errors on inverted CO 2 surface fluxes from OCO measurements. Geophysical Research Letters, American Geophysical Union, 2007, 34 (24), ff10.1029/2007GL030463ff. ffhal-02948201f

Tang, J., Zhuang, Q. (2008). Equifinality in parameterization of process-based biogeochemistry models: A significant uncertainty source to the estimation of regional carbon dynamics. Journal of Geophysical Research, 113, G04010. https://doi.org/10.1029/2008JG

Ziehn, T., Scholze, M., and Knorr, W.: On the capability of Monte Carlo and adjoint inversion techniques to derive posterior parameter uncertainties in terrestrial ecosystem models, Global Biogeochem. Cy., 26, GB3025, https://doi.org/10.1029/2011GB004185, 2012.

Thanwerdas, J., Saunois, M., Berchet, A., Pison, I., Vaughn, B. H., Michel, S. E., and Bousquet, P.: Variational inverse modelling within the Community Inversion Framework to assimilate 13C(CH4) and CH4: a case study with model LMDz-SACS, Geosci. Model Dev. Discuss. [preprint], https://doi.org/10.5194/gmd-2021-106, in review, 2021.

Santaren, D., Peylin, P., Bacour, C., Ciais, P., and Longdoz, B.: Ecosystem model optimization using in situ flux observations: benefit of Monte Carlo versus variational schemes and analyses of the year-to-year model performances, Biogeosciences, 11, 7137–7158, https://doi.org/10.5194/bg-11-7137-2014, 2014.

Bacour, C., et al. (2015), Joint assimilation of eddy covariance flux measurements and FAPAR products over temperate forests within a process-oriented biosphere model, J. Geophys. Res. Biogeosci., 120, 1839–1857, doi:10.1002/ 2015JG002966.