

Interactive comment on “CH₄ parameter estimation in CLM4.5bgc using surrogate global optimization” by J. Müller et al.

Anonymous Referee #2

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In this paper, the parameters of a complex simulator are optimized by applying surrogate based optimization techniques to minimize the error on a set of real observations at distinct geographical locations. The organization and presentation of the paper is very good, and the problem that is solved is real and significant. In addition, a clear motivation for the usage of surrogate based optimization instead of traditional gradient based optimization approach is given. I have two concerns that require some clarification and a question:

- The applied screening mechanism evaluates the change in output behaviour by changing inputs values locally to the default values and will therefor select the parameters responsible for significant output variability in that part of the parameter space. The excluded parameters potentially influence output variability further away from the

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default values. Furthermore, the screening does not take into account possible interaction effects of parameters although the authors mention in section 5.1.2 the CLM effectively makes use of interactions. Therefor I'm not convinced the applied method produces the best feature ranking. Perhaps methods such as Elementary Effect [1] or Locating Arrays [2] may identify a different subset of features.

- The authors correctly re-weight the error contribution of each site to avoid biased results as an absolute error function is used. Also they mention the different sites are geographically varying but does this guarantee all sites differ significantly? If some sites are related at the level of the data (in other words, representing the same part of feature space) it means that group starts to dominate the error function. My opinion is some additional information on the diversity amongst the sites at the level of the data is needed (for instance by clustering the union of all observation data), to provide proof that the relative contribution of each site to the total error should be equal.

- From the results and the discussion on the real data it seems there is a difference between methane production in northern and southern regions. Have the authors considered applying multi-objective surrogate based optimization [3] to identify a set of pareto-optimal configurations? Having 16 independent objectives is perhaps too much, but splitting the sites in two groups (northern, southern) and computing a weighted RMSE as in Equation 1 for both could result in several distinct solutions of which some are more suited for different regions.

Technical remarks: - Although it may be implied, is the applied simulator deterministic (producing the same value for a combination of input parameters everytime)? - Equation 2 should be part of Equation 1.

[1] Campolongo, Francesca, Jessica Cariboni, and Andrea Saltelli. "An effective screening design for sensitivity analysis of large models." *Environmental modelling & software* 22.10 (2007): 1509-1518.

[2] Aldaco, Abraham N., Charles J. Colbourn, and Violet R. Syrotiuk. "Locating Ar-

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rays: A New Experimental Design for Screening Complex Engineered Systems." ACM SIGOPS Operating Systems Review 49.1 (2015): 31-40.

[3] Couckuyt, Ivo, Dirk Deschrijver, and Tom Dhaene. "Fast calculation of multiobjective probability of improvement and expected improvement criteria for Pareto optimization." Journal of Global Optimization 60.3 (2014): 575-594.

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