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Interactive comment on "Optimization of experimental designs and model parameters exemplified by sedimentation in salt marshes" *by* J. Reimer et al.

Anonymous Referee #1

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General comments:

The paper discusses methods for nonlinear experimental design and their application to a case-study from geoscience. The results show improvements of model accuracy while at the same time saving experimental costs.

The reviewer suggests publication of the paper after the revisions discussed below.

Three major remarks:

1. For a paper in a geoscience journal, a main focus of the paper should be on the application. They should be discussed in the beginning of the paper addressing the

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interests of the readers of the journal. At the moment the geoscience application first appears in Chapter 4.

2. Is it aim of this article to give a documentation of the Optimal Experimental Design Toolbox? This should be described in some other paper. Chapter 3 should be less technical.

3. Some explanations and conclusions in Chapter 4 on the numerical results should be reconsidered. For details see below.

Minor comments:

p 6442ff: Say "estimation of model parameters" instead of "optimization ..."

p 6442f: Choice of the estimator: the estimator should be derived from the statistical properties/distribution of the measurement errors, e.g. a maximum likelihood estimator

p 6442: Set of feasible model parameters, described by bounds: what is the use of an estimate if the bounds (which have been specified by the modeler) are active?

p 6443: Can psi be assumed to be injective?

p 6443: Use of SQP for PE is not really a good idea, for large residuals it may converge to statistically unstable solutions, see Bock et al. 2013 better use Gauss-Newton For exp. design SQP is ok.

p 6443 l 24: "normally distributed"

p 6443f: What are the regularity assumptions? E.g. for the inverse of Mn(p) it is: nabla_p fˆT has full (column) rank.

p 6445 l 23-13: The operation "set to infinity" is not differentiable, which is needed for application of SQP.

p 6446: Experimental design: what about optimizing the x_i?

p 6447 l 2: "occur nonlinearly"

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p 6447 l 24: typo: can be solved

p 6449 l 19: For derivative based optimization of the exp design problem, e.g.. by SQP, a mixed derivative is required to compute the gradient of the objective.

p 6450 l 21: "initial guess" instead of "initial estimation"

p 6457 l 26: "normally distributed"

p 6458 l 11ff: If you also use the high water levels of the tidal inundation as experimental design variable, you need derivatives wrt. this quantity for the SQP optimization. How do you compute them? (In contrast, derivatives wrt. the w_i only need nabla f.)

p 6459f: The phrase "maximal accuracy" is misleading. Of course the accuracy can always be improved further by performing additional measurements.

p 6459f: Which gamma did you choose in the robust approach? How big is the standard part of the objective compared to the robustification part?

p 6459ff: Conceptionally, the relaxed solution should be better than the discrete one, because the feasible set is larger, Unless you compare local relaxed to global discrete minima which is not a fair comparison.

p 6459 l 12: typo: worst -> worse

p 6459 l 15: "occur nonlinearly"

p 6459 l 22f and p 6460 l 16f: This is because here the different (constant) standard deviations only mean a different scaling of the objective of the exp. design opt. problem. Only if the stqandard deviations are non-constant within the experiments, the weighting by 1/sigma becomes relevant.

p 6460 l 24: replace greater by bigger, e.g.

p 6460 l 27f: This explanation sounds weird. See remark above. The behavior should depend on the actual nonlinearity of the problem.

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p 6462 l 14ff: This kind of results also occurs for linear models. This may indicate why the robust approach is not needed.

p 6472: Fig. 2: 1.input should be the "RHS of the differential equation".

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