**Geoscientific
Model Development
Discussions**

Interactive comment on "Using model reduction to predict the soil-surface C^{18}OO flux: an example of representing complex biogeochemical dynamics in a computationally efficient manner" *by* W. J. Riley

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Response to reviewers' comments on "Using model reduction to predict the soil-surface C18OO flux: an example of representing complex biogeochemical dynamics in a computationally efficient manner" by W.J. Riley.

Below, I respond to the comments by the two reviewers of this paper. I put the reviewer comments in regular font, and my responses in italics.

Anonymous Referee #1 The author applies a high-dimensional model representation

(HDMR) approach to a model of the isotopic flux of CO2 from the terrestrial biosphere (ISOLSM). He demonstrates that the model is well capable to reproduce the full ISOLSM at a C4 grassland. The paper is short, concise and sound. I have only the obvious remarks about predictability, etc. Additionally, the paper needs more explanations about quite a few concepts mentioned and or applied, that might or might not be important, but are not elaborated upon. 1. What is steady-state in this context? Steady in what? If I force ISOLSM with random precipitation input, diurnal and seasonal cycles of temperature, etc., when is it steady? *For a steady-state soil moisture content, CO2 production, and 18O content of soil moisture, the 18O content of the surface CO2 flux is uniquely determined. However, as the reviewer states, there are many time scales of variability in the system that will force these precursor states, and therefore the resulting surface flux, away from equilibrium. My point in the discussion of steady-state in the manuscript is to indicate that, under the variability associated with climate at this site, excursions from steady conditions do not result in large excursions of the soil-surface C18OO flux. Therefore, the use of the HDMR functions developed under steady conditions is appropriate for accurate prediction (see discussion on page 3478, lines 20-25).*

2. What is the predictive power of the HDMR? What happens far away from steadystate (but see 1)? What happens outside the parameter ranges that were used for the sampling points of HDMR. *The impact of the steady-state assumption was tested and demonstrated in Figure 2 and the calculation of the impact on the cumulative isoflux (< 0.2%; page 3480, line 15). The parameter ranges were carefully chosen and include realistic values. However, I would expect potentially larger errors if the HDMR solution were applied outside of the parameter ranges for which it was developed.*

3. What is the advantage of HDMR over artificial neuronal networks (ANN) or other similar approaches? *I have added a citation to analyses that have coupled ANN with HDMR. The reported advantages include decreased computational requirements for higher dimensional problems than that attempted in the current manuscript.*

4. The model was built for the isotopic flux. If I am interested in other things than the flux, I still have to run the full model, isn't it. I thought that isotopes are a diagnostic tool and, therefore, am I not always interested about other things on top of the isotopic fluxes? I just have a problem to imagine a scenario where I am interested in only the fluxes. The fluxes are to and from the atmosphere. Atmospheric isotopes are used for double deconvolution, for example. But then I also need the fractionations. Could the author please further explain what the HDMR of ISOLSM is needed for. Would it be possible to build (an) HDMR but with several output variables, e.g. also the fractionation factors? The atmospheric inversions often require either a fractionation (which can be calculated from the surface C18OO and CO2 fluxes) or the flux itself (C18OO). These inversions typically don't require detailed information of, e.g., the 18O content of CO2 in the soil pore space. So, the HDMR solution provides a computationally efficient and accurate method to provide the atmospheric inversions the information they need. And, yes, it's possible to build the HDMR solution with multiple output variables.

5. I cannot believe that Table 1 lists all relevant inputs to build the HDMR. Or put it another way, I think that there are more relevant parameters that were not used in HDMR but are important in ISOLSM. One obvious missing parameter is porosity, another one is CO2 concentration. This might hinder the predictive skills. Moreover Table 1 is not indicating which soil moisture and temperature were taken: in one depth, the same in all depths, etc. Consequently I wondered if the remaining parameters in ISOSLM were fixed at the values for the C4 prairie where the model is validated now. 1. The reviewer is correct that other variables are used in ISOLSM to specify conditions at the site that are then used in the simulation to prognose the variables in Table 1. However, those variables are not used to generate the expansion functions, which is the purpose of Table 1. As long as those values are provided at any particular site, the HDMR solution can be calculated. This point is alluded to on the top of page 3475; I have clarified this point in that sentence. 2. As indicated in the Table caption, the variables that are depth-dependent are taken at either 2.5 or 5 cm control volumes. 3. Yes, the example here is taken from the prairie site for which the model was tested

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in this manuscript. As mentioned above, the values in Table 1 fully define the input parameters for the HDMR simulation.

6. I have not understood the business of D1 and D2. This was not well explained. On page 3476, lnes 7-12, I describe the two vertical discretization scenarios. Basically, ISOLSM is a vertically resolved reactive transport solver, and it can be discretized at user discretion. Using these two discretization scenarios I demonstrated the relative importance of resolving the near-surface 18O and bulk soil moisture gradients (see e.g., Figure 3 and text on page 3478).

7. The author uses cut-HDMR and linearly interpolated between the forcing values. He therefore chose small steps. I wondered why he did not use (random sampling) RSHDMR using quasi-random numbers and orthogonal interpolation functions. Would that not decrease build-up time of the HDMR enormously? It might even reduce the computation time again. The reviewer is correct that there are other methods to sample the model phase space, and that one of the other methods might provide even better computational efficiency then demonstrated here. I chose the cut-HDMR approach because the phase space covered by the input variables is large and relatively homogeneously populated, and because that method is relatively easy to implement. To address the reviewer's concern, I have added text to the Methods section citing the RS-HDMR approach.

Anonymous Referee #2 Received and published: 21 January 2013 This manuscript presents an application of the High-Dimensional Model Representation (HDMR) in an isotopic model of soil CO2 fluxes. The approach greatly decreases computational time and is of valuable use for integrating soil isotopic fluxes in more complex Earth system models. The paper is interesting and the application of this methodology should also interest model developers in other branches of Earth system modeling. However, I feel the manuscript does not provide enough detail to reproduce the results or exemplify the use for other applications. I believe this additional information would greatly improve the value of this contribution and would make it more suitable for publication in

Geoscientific Model Development.

Specific comments - One of the main objectives of Geoscientific Model Development is to provide detailed model descriptions that ensure their reproducibility. The journal encourages the submission of source code and user manual, so the model or the technical aspects presented in the manuscript can be evaluated or reproduced. I encourage the author to provide additional details about his contribution, e.g. link to source code and user manual, or pseudo code that can be used as template for reimplementation. I would be happy to contribute the Matlab code I used to generate the HDMR functions and to evaluate the system's dynamic response. Perhaps the editors can inform me on how to do this.

- The ISOLSM model needs to be described in more detail. Model description in this case is important for the reader to understand the level of complexity and nonlinearity of the model, and therefore get an understanding of the advantage of the HDMR. Although the model is already described in Riley et al. (2002), it'd be very useful if you provide a list of the main equations, or the phase-space dimension, number of variables, parameters, etc. The ISOLSM model is relatively complex, so I deferred the readers to the detailed description in Riley et al. (2002) and the eleven other papers in which the model has been applied. The details on ISOLSM mechanisms given on pages 3473 and 3474 should provide the reader with sufficient information to interpret the HDMR results presented in the current manuscript, which is the main goal of this GMDD paper.

- In section 2.3. you point out that the HDMR methodology was applied to a solution of the ISOLSM model at steady-state. What do you mean by steady-state in this nonlinear model? Have you studied the dynamical behavior of this model? Is it possible that by changes in parameter values the stable 'steady-state' solution drifts to a non-stable or cyclic solution (bifurcations)? Perhaps it would be helpful if in the model description section you mention the expected dynamic behavior of the system and whether the 'steady-state' is a stable node or cyclic behaviors are possible. This information would

help the reader to understand whether the HDMR methodology may have limitations for special cases of nonlinear dynamics. See the responses #1 and #2 to a similar concern by Reviewer #1.

- The discretization scenarios are very helpful to evaluate possible numerical error. Would it be possible to make a more general statement about the effect of discretization on the error of the predictions? For example, does the error decrease linearly with depth increments (discretization size)? To clarify, the differences in D1 and D2 were not evaluated to infer numerical errors in the underlying ISOLSM model (which is run at the higher resolution), but to evaluate errors in the HDMR approach associated with averaging the ISOLSM solution to the coarser resolution. A more general statement about the impact of averaging on the HDMR solution is outside the scope of this paper, and probably not necessary since I demonstrate that one needs to resolve the gradients seen in the 2.5 cm resolution model.

Technical comment - The first three paragraphs presents very basic information not necessarily needed for this manuscript. Perhaps you can reduce the length of the introduction by merging some of the ideas of the first three paragraphs into a single one. I feel that the relatively small amount of information given in these paragraphs is important to provide a context for the modeling exercise, and to justify the particular problem being analyzed and the application of the HDMR technique.

- Page 3473, line 20. above canopy water vapor? The model requires boundary conditions at the top of the canopy, and atmospheric water vapor content above the canopy is one important BC.

- Page 3474, line 1. What is V-SMOW? Both V-SMOW and V-PDB-CO2 are standards used to evaluate the ïĄď values calculated by the models and observed in the field; I have clarified these definitions in the revised manuscript.