**Summary until now.**

This week I have been able to couple an optimization algorithm to the model to select the best combined Nash for **soil**concentrations and isotope data by testing only two parameters (i.e the reference DT50 and the Epsilon value).

The first purpose for doing this was trying to get a rough idea of what would be the best Nash that we may expect from a complete parameter search (i.e. assuming degradation parameters are the key regulators of pesticide fate).

The second purpose is to evaluate the last structural model decision to make. That is, remember that for this optimization test the actual DT50 is considered as dependent on moisture and temperature conditions. However, there are two ways of controlling this dependence (i.e. Schroll or Walker). How DT50 changes under each is attached as heat maps. The current optimization run (since this morning) is testing the model for Schroll. I will test tonight Walker and compare the optimization results for each. I will then choose the one yielding the best soil Nash value.

**Revisiting the Paper Questions**

Answering Q1 and Q2 below will be approached by the following procedure of analysis:

Step 1. Obtaining the parameter ranges of the best fit models (i.e. those falling above a certain Nash criteria)

Step 2. Define the Nash criteria for the current question (Q1 or Q2)

Step 3. Compare parameter range-reduction from models tested and selected based on Nash criteria.

**Q1:  *Can consideration of climatic variations in soils improve reproduction of pesticide fate and degradation extent?***

- Compare parameter ranges from models with fixed DT50 (mod1) vs variable DT50 (mod2)

- Select the models defining the parameter range based on Nash1 and Nash 2

* *Nash1 (soil concentrations)*

The Nash1 is obtained from models with a constant DT50, and thus no need for outlet discharge (as controlling variable for catchment moisture conditions is needed or relevant).

* *Nash2 (soil conc + outlet discharge)*

The Nash2 is obtained from models where DT50 is moisture/temperature dependent, and for which outlet discharge is a required constraint (and thus data also a Nash-equation input).

**Answer**: Did we reduce parameter uncertainty with mod2?

***Doubt:****Is outlet discharge a good enough constraint for soil moisture. Maybe to discuss in limitations, but a potential defense here would be to compare Nash values of both models but only for soil conc. and see if the second model can reduce uncertainty even without considering outlet discharge as a constraint.*

***Q2: What is the added value of CSIA?***

Compare parameter ranges from the same model (mod2 above), but applying different Nash criteria to select which models determine parameter ranges.

* Nash2 (same as above, soil conc + outlet discharge)
* Nash3 (soil conc + isotopes + outlet discharge)

**Answer**: Did we reduce parameter uncertainty with mod2 and isotope data?

***Q3. What is the added value of 2D models?***

- First, I think it is important here to mention that the limits of a model go hand in hand with the data used to constrain it. As such, we then reiterate the value of CSIA in reducing uncertainty and model adequacy in providing more accurate information to the user.

- The model demonstrated here that spatial and temporal variability are in fact important in regulating pesticide degradation. This was done by the ability to reduce parameter uncertainty by inclusion of a variable DT50 (i.e. Answer to Q1).  Here we could note that although we evaluated only soil moisture and temperature, additional factors such as soil composition or bacterial communities are also likely to be key regulating factors that should be accounted to further reduce uncertainty.

- A final point could be made in terms of exploring the variability of epsilon values to see if we can explain what Fatima saw in her experiment. Here the model could be used to plot the uncertainty ranges / variations of epsilon values associated to the best models as a function of temperature or moisture. Can we answer: Is there more/less uncertainty in epsilon values at certain temperature/moisture ranges? Hypothesis: Expect less variation at sub-optimal (i.e. extremes) growing conditions. Not sure if these variations will be significant, need to check.

**Q4. Expected changes of near and far future climatic variables.**

- Subject to interesting answers to questions Q1-Q3.

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**Visuals**

What visual results do we need to answer Q1 – Q3?

**Main text - Results**

Fig. 1 -> Concentrations and isotope data **on soils** temporal and spatial dynamics. Similarly to Lutz, we could overlap model output ranges showing how predicted values may be narrower for the more complete model.

Fig. 2 -> I would propose a set of histograms depicting parameter ranges (namely DT50 and epsilons and other parameters with significant reduction in uncertainty across models/criteria). I would like it if I can find a way to overlap the three histograms per parameter shown, with the largest range at the back.

Fig 3. -> Plot of DT50 and epsilon variability as a function of moisture and temperature (see answer to Q3 below)

**SI.**

Fig 1 -> x:y graphs for the appendix, showing how different models perform and yield different Nash values.

Fig. 2 -> Heat maps for showing how Schroll and Walker affect the DT50. Explaining that Schroll (or Walker) was chosen due to optimal fitting before running GLUE tests.

**What are the next steps?**

- Define parameters to test (attached as excel,will follow tomorrow)

- For each parameter, define a range to test (proposed on the excel)

- For each parameter, determine if the distribution should be normal or uniform **(to be decided next meeting for each parameter)**, so that we can create the parameter sets to run a Monte Carlo simulation from a sampling set.

- Define how Nash will be computed:

**- i.e. how to combine observation types? Do we weigh or not?**

- Choose a minimum Nash criteria to select 95% of the best models.