Quantifying global air-sea fluxes of N_2O by the inversion of oceanic observations

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1 Motivation and background

The first part of my Ph.D. project involved compiling a global data base N_2O data, which we want to use to quantify global air-sea fluxes of nitrous oxide by using inversion techniques. For an introduction to inverse modelling I visited the working group of Nicolas Gruber, who is one of the leading experts on inverse modelling.

2 Summary

During my visit, I was introduced to the underlying scientific ideas and mathematical concepts of inverse modelling:

The world ocean is divided into n regions, $n \in \mathbb{N}$, the extent of which depends on the available data set and its ability to resolve the differences between regions and every region is associated with a flux (or flux pattern) of a given tracer. For each region a global circulation model is used to propagate the associated flux through the global (assuming there are no other source terms). The model is then run forward in time until is reaches a quasi steady state. The resulting global distribution constitutes the respective base function.

The observed concentration of the tracer $conc_{\text{tracer}}$ at any given point in the ocean should then equal a linear combination of the n base functions, i.e.

$$conc_{\text{tracer}} = \sum_{i=1}^{n} \lambda_i f_{n_i}, \ \lambda_i \in \mathbb{R}.$$

Fitting the modelled concentration to the observations in a least squares sense effectively means solving the stated inverse linear problem for $\lambda = (\lambda_1, ..., \lambda_n)$.

Using the solution vector λ you can then calculate the regional fluxes which probably created the observed concentrations by multiplying λ_i with the respective original flux patterns.

The general scheme introduced above only works for conservative tracers since it does not take any sources or sinks in the ocean interior into account. Nitrous oxide is biologically produced and decomposed so this issue needs to be addressed.

We used the approached suggested by Jin & Gruber [1] to constrain the production mechanisms. They assumed two production pathways:

- a nitrification pathway

  $$J^{\text{nitr}}(\text{N}_2\text{O}) = \alpha \ r_{N:P} \ J(\text{PO}_4^{3-}),$$

  where α is a scaling factor and the symbol $r_{N:P}$ is the N to P ratio of organic matter (assumed to be 16:1).

- a low oxygen pathway

  $$J^{\text{low-O}_2}(\text{N}_2\text{O}) = \beta \ f(\text{O}_2) \ r_{N:P} \ J(\text{PO}_4^{3-}),$$

  where β is a constant and $f(O_2)$ is a a slightly modified version of the function of the in situ oxygen concentration given by Suntharalingam & Sarmiento [2].

They then used interior sources (per region) described by the respective production pathways and a constant global decomposition term instead of prescribed flux patterns to calculate the respective base function. These were calculated coupling the Princeton OCMIP model (Modular Ocean Model version 3) with a biogeochemical model and the production/decomposition model explained above.

Using these base functions and some exemplary MATLAB code I developed - with support from Kay Steinkamp - a suite of MATLAB functions tailored to the existing base functions and my data base to calculate inversions during my stay in Zurich.
While it is comparatively simple to calculate such inversions (from a mathematical point of view) the parameters need to be finely tuned to obtain optimal and meaningful results.
Model results, for example, are given on a grid (which pertains to the model). In order to compare observations and calculated concentrations the observations need to be binned to the model grid. As there can be boxes with more than one observation (likely in a coarse resolution global model) one needs to think about a sensible weighting of these "multiple" observations.
Also, it might make sense to add additional constraints to the system of linear equations. In case of the two production pathways it seems reasonable to force λ_i to be non-negative (as consumption is modelled in a different way and taking into account the way they are modelled none of the two processes can switch to decomposition).

Care has to be taken in preparing the observational data to be used in the inversions. In the special case of N_2O parametrisation of the production heavily depends on the oxygen concentration calculated by the model. Since I learned in Zurich that most global-scale biogeochemistry models still show significant deficiencies in reproducing suboxic and/or anoxic zones it is important to keep this in mind.
In terms of data preparation it means that we decided to exclude data from the Baltic Sea since it is very unlikely that a coarse resolution model is able to reproduce its erratically oscillating oxygen content. There is also a relatively large amount of uncertainty concerning other marginal seas, so maybe we need to discard data from the Mediterranean as well. This is still being discussed.

One workaround for the oxygen problem is to use "real" observed oxygen data to calculate the amount of produced nitrous oxide , since was also suggested before by Jin & Gruber [1] and the relevant base functions have been calculated and will be used.

In the framework of a group seminar, I also had the opportunity to present my research to the work group of Professor Gruber. The talk was titled "Nitrous oxide – data and measurement techniques".

3 Future work

Planned future work includes:

- Short term:
    - implementing a sensible weighting to the observations implementing the calculation of additional diagnostics as, for example, the resolution matrix and the condition matrix, which contain information about how distinct (i.e. in a sense "well-defined") the respective base functions are.
    - implementing other side conditions (e.g. $\lambda_i \geq 0$) optimise the graphical output of the MATLAB routines to facilitate a more intuitive and comprehensive analysis of the results
    - use the different base functions (real oxygen/modelled oxygen)
    - calculate air-sea fluxes once the production mechanisms are adequately constrained
- Medium term:
    - recalculate base functions using (a) different circulation model(s) to test the robustness of results and find suitable confidence intervals for calculated fluxes

We are planning for Kay Steinkamp to come to Kiel for a return visit in order to facilitate the planned future work.

References

[1] Jin, X. and Gruber, N., *Constraining N_2O production mechanisms*, manuscript.

[2] Suntharalingam, P. and Sarmiento, J. L., *Factors governing the oceanic nitrous oxide distribution: Simulations with an ocean general circulation model*, Global Biogeochemical Cycles, 14 (1), 2000, pp. 429-454, 0886-6236.