We investigate the performance of an existing mesocosm-based ecosystem model developed by Schartau and co-workers (Biogeoosciences, 2007), which allows for a decoupling of carbon and nitrogen dynamics (CN_RecoM; cf. fig. 1). The model is extended to resolve calcification by including an extra phytoplankton component, Emiliania huxleyi (coccosphere in fig. 1). Based on the findings of Schartau, Hohn et al. (EPOCA deliverable D9.4), calcification rate is calculated as:

\[
\text{Calc.} = a \text{ DIC} / (b \text{ DIN} + c \text{ PO}_4 + d \text{ DIC})
\]

E. huxleyi is assumed to have a constant PIC:PICO ratio of 0.47. To assess the robustness of the model it was fitted to two different mesocosm datasets. The original model was fitted to data from an experiment described by Engel et al. (Limnology & Oceanography, 2002). The extended model is being tested using a second dataset from the first Pelagic Ecosystem CO2 Enrichment (PeECE I) experiment (Engel et al., Limnology & Oceanography, 2004).

The model is written in Fortran and investigated using the FME package in the statistical software R (R Development Core Team, 2010; Soetaert & Petitzko, 2010). Using datasets from different mesocosm studies, the overall robustness of the model structure and parametrization is evaluated.

1a. Model fit to the original mesocosm data
Calcification was switched off while fitting the model to the original mesocosm dataset. Besides the variables shown below DON, DOC, and TEPC (transparent exopolymeric carbon) data were available. The model fitted the data well, apart from an overestimation of the chlorophyll a concentration (fig.2).

1b. Model fit to the PeECE I data
The extended model, with calcification switched on, was fitted to the PeECE I dataset (current CO2 conditions). This dataset contained additional data on the carbonate system, particulate inorganic carbon, total alkalinity, pH, phytoplankton numbers and nutrients.

2a. Local model sensitivity to the original parameters
Not all parameters can be optimized (at the same time), and for some parameters changing the values does not necessarily alter the goodness-of-fit (model cost) of the model to the data (i.e. the model is insensitive to these parameters). Therefore, model fitting is an iterative process of choosing appropriate parameter sets by local sensitivity analysis and identifiability analysis, followed by the actual fitting of the chosen parameters.

Local model sensitivity reflects responsiveness of model (output variables) to small changes in a particular parameter.

* The CN_RecoM model is sensitive to initial conditions (…int.; fig.4).
* C-specific photosynthesis rate (p_c) is important for optimization.

Variable sensitivity can be investigated over time (fig.5):
* Sensitivity of variables is not constant over time.
* Strong similarity in time dependence for different parameters. (makes that parameters may be difficult to estimate together)

2b. Local model sensitivity to the PeECEI parameters

* Initial conditions are also important in the extended model (fig.6a). (measurement deserves much attention)
* Model is insensitive to large fraction of parameters (fig.6a) (but local sensitivity >> things are different after optimization)
* Model is not sensitive to calcification parameters (fig.6a and b) (model cost does not change over wide range of parameter values)

Model sensitivity to parameters a. Here the C-specific photosynthetic rate of the coccolithophores is included (p_c_CocCo). Variable sensitivity for particulate PIC and dissolved DIC inversely correlates with regard to the calcification parameters (see above).
* Model sensitivities with regard to different parameters are strongly correlated (fig.7a).
* A change in one parameter can be compensated by a change in another parameter (overparameterization)
* The collinearity index indicates how strongly changes in parameters are linearly related (fig.7b). A parameter combination with indices above 15 is almost certainly not optimizable. Lower indices might be optimizable or non-linearly related...

3. Preliminary results:
Local sensitivity analyses and identifiability analyses have pointed out that the CN_RecoM model is not easily fitted to any set of mesocosm data. Different parameters require different subsets of data to fit. Many parameters show too much mutual dependence to be fitted simultaneously. However, despite the dominance of certain parameters in the model sensitivity (cf. p_c), the order of importance of others differs with dataset, implying a certain flexibility in the model, but also a need for elaborate knowledge on parameters that cannot be estimated. This emphasizes the need to investigate models for their robustness with regard to different datasets (and natural conditions).

Future perspectives:
- Assessment of the uncertainty in model output, given the inputs and data-based parameter estimates (global sensitivity analysis using Markov-Chain-Monte-Carlo approaches).
- Provide information to experimenters on which information on initial conditions and data for fitting are needed.
- Improve model performance with regard to running time, and resolving calcification.

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