# OPTIMIZATION AND VALIDATION OF BIOGEOCHEMICAL MODELS

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In the framework of aquatic ecosystems studies, the determination of exchange rates between different nutrient reservoirs is of crucial importance for the understanding of biogeochemical cycles. In this study quantification of the exchange rates based on stable isotope tracer experiments is investigated. In order to extract values for the flux rates from these measurements, it is necessary to postulate a model and, if required, to choose an appropriate optimization method. The numerical values will largely depend upon the criterion and method used to match model and measurements. The aim of this work is to make a rigorous contribution to the estimation of flux rates, allowing to issue statements about the result uncertainty for both random and systematic errors. A series of models is considered, describing both the silicon and nitrogen cycling in aquatic systems.

In a first step, the cost function concept is introduced. A cost function expresses the goodness of fit between measurements and postulated model. The optimal parameters (here they represent flux rates) thus correspond to a minimal cost function. Least Squares and Weighted Least Squares cost functions are two classical examples. Since in our case experimental uncertainties are known, the Weighted Least Squares method is preferred: (i) it provides a more reliable estimation, and (ii) the residual cost function value can be interpreted, thus providing additional information concerning the significance of the difference between model and measurements. For instance, one examined experiment has been identified as an outlier, although it was not yet compared to any other measurement. When the method is applied to a whole data set of 53 experiments, two other outliers are unmasked. Moreover, an overall statistical analysis reveals that the experimental uncertainties, provided by the experimentalist, are overestimations of the real ones.

In the second part, the Weighted Least Squares procedure and its underlying assumptions are validated on simulations. Some weaknesses of the estimator are illustrated. An improvement is proposed, based on taking both input and output experimental uncertainties into account. This procedure appears to offer better results, especially to quantify the uncertainty on estimated flux rate values.

Finally, a new optimization method is presented, based on Interval Analysis. Whereas most methods use local optimizations, this approach is able to guarantee that the parameters found correspond to all the global minima the cost function possesses. This allows a unique reliability of the solutions. The method was applied to several nitrogen models in order to determine whether the solution loci associated with the model are uni- or multi-modal. One unreliable model was revealed, which was proved to be useless for precisely determining flux rates.