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A new mathematical approach for modeling biogeochemical consumption and production rates from measured vertical concentration profiles in aquatic systems

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A numerical procedure is proposed which allows the estimation of microbiological consumption and production rates from measured nutrient and metabolite concentration profiles in limnic and marine sediments. The basis of the estimation process is based on the one-dimensional steady state diagenetic transport-reaction equation for dissolved compounds. This equation is inverted by a technique called Tikhonov regularization which is a common and robust technique for solving ill-conditioned inverse problems.

The procedure is tested with artificial test cases and real measurements of sulfate profiles. Furthermore, the technique is compared with results obtained from the PROFILE model of Berg et al. (1998) and the model of Wang et al (2008), which is very similar to the PROFILE model. The both models are a widely used and are also very robust in estimating consumption and production rates via a different procedure from measured vertical nutrient concentration profiles.

From our model results, it can be concluded, that the proposed numerical procedure is suited to estimate robust and reasonable rate profiles if the relative measurement errors are not larger than 5-10%. In the case of larger measurement uncertainties, at least a nearly constant mean rate profile can be estimated.