Geophysical Research Abstracts
Vol. 12, EGU2010-11675, 2010
EGU General Assembly 2010

Information content of incubation experiments for inverse estimation of pools in the Rothamsted carbon model: a Bayesian approach

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Turnover of soil organic matter is usually described with multi-compartment models. However, a major drawback of these models is that the conceptually defined compartments (or pools) do not necessarily correspond to measurable soil organic carbon (SOC) fractions in real practice. This not only impairs our ability to rigorously evaluate SOC models but also makes it difficult to derive accurate initial states. In this study, we tested the usefulness and applicability of inverse modeling to derive the various carbon pool sizes in the Rothamsted carbon model (ROTHC) using a synthetic time series of mineralization rates from laboratory incubation. To appropriately account for data and model uncertainty we considered a Bayesian approach using the recently developed DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm. This Markov chain Monte Carlo scheme derives the posterior probability density distribution of the initial pool sizes at the start of incubation from observed mineralization rates. We used the Kullback-Leibler divergence to quantify the information contained in the data and to illustrate the effect of increasing incubation times on the reliability of the pool size estimates. Our results show that measured mineralization rates generally provide sufficient information to reliably estimate the sizes of all active pools in the ROTHC model. However, with about 900 days of incubation, these experiments are excessively long. The use of prior information on microbial biomass provided a way forward to significantly reduce uncertainty and required duration of incubation to about 600 days. Explicit consideration of model parameter uncertainty in the estimation process further impaired the identifiability of initial pools, especially for the more slowly decomposing pools. Our illustrative case studies show how Bayesian inverse modeling can be used to provide important insights into the information content of incubation experiments. Moreover, the outcome of this virtual experiment helps to explain the results of related real-world studies on SOC dynamics.