Forward Modeling the Alkenone paleo-CO₂ Proxy: Combining Traditional Approaches in a Bayesian Framework

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Stable carbon isotopes (δ^{13} C) in phytoplankton have long been used to reconstruct atmospheric CO₂ over geologic timescales. , as the photosynthetic fractionation of carbon isotopes (ε_p , the difference between aqueous CO₂ and organic C biomass) positively correlates with [CO₂]_{aq} due to kinetic rate differences in the transport and fixation of ¹³CO₂ and ¹²CO₂. However, non-[CO₂]_{aq} effects on ε_p , including variation in growth rate and cell geometry, complicate interpretation of the proxy data. Several strategies to incorporate these effects have been developed, including: (1) corrections based on empirically calibrated relationships with [PO₄³⁻] in the modern ocean[1], (2) modifying [PO₄³⁻]-based corrections to account for differences in cell geometry[2], and (3) using cell size estimates to account for both growth rate and geometric effects[3].

Here, we present a forward Proxy System Model (PSM) to reconcile these three approaches. We couple an established theoretical model of the physiology and biochemistry underlying $\varepsilon_n[4]$ with prior estimates and observations of $[PO_4^{3-}]$, cell size from coccolith length, and other environmental parameters. Because phytoplankton growth rate, cellular carbon content, and surface area-the factors that collectively determine the non- $[CO_2]_{a0}$ correction—are linked to both $[PO_4^{3-}]$ and coccolith size, the model combines the information (and the associated uncertainty in a given application) inherent in all three approaches described above. We implement the PSM in a Bayesian hierarchical framework and explore the implications of modern empirical data and paleo-records on the posterior distributions of the full suite of model parameters. Comparison of these modern (spatial) and temporal results are used to assess the stability of the method across different calibration regimes and with different data constraints. We evaluate the performance of the PSM-based approach relative to the 'traditional' methods and assess the implications of our results for the use of mechanistic models in the interpretation of paleo-proxy data.

[1]Pagani et al., 2002, Phil. Trans. Roy. Soc.; [2]Hendericks and Pagani 2007, Paleocean.; [3]Zhang et al., 2020, GCA; [4]Rau et al., 1996, Marine Ecology Prog. Series