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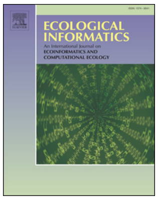

Beyond the benchtop and the benthos: Dataset management planning and design for time series of ocean carbonate chemistry associated with Durafet®-based pH sensors

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ABSTRACT

To better understand the impact of ocean acidification on marine ecosystems, an important ongoing research priority for marine scientists is to characterize present-day pH variability. Following recent technological advances, autonomous pH sensor deployments in shallow coastal marine environments have revealed that pH dynamics in coastal oceans are more variable in space and time than the discrete, open-ocean measurements that are used for ocean acidification projections. Data from these types of deployments will benefit the research community by facilitating the improved design of ocean acidification studies as well as the identification or evaluation of natural and human-influenced pH variability. Importantly, the collection of ecologically relevant pH data and a cohesive, user-friendly integration of results across sites and regions requires (1) effective sensor operation to ensure high-quality pH data collection and (2) efficient data management for accessibility and broad reuse by the marine science community. Here, we review the best practices for deployment, calibration, and data processing and quality control, using our experience with Durafet®-based pH sensors as a model. Next, we describe information management practices for streamlining preservation and distribution of data and for cataloging different types of pH sensor data, developed in collaboration with two U.S. Long Term Ecological Research (LTER) sites. Finally, we assess sensor performance and data recovery from 73 SeaFET deployments in the Santa Barbara Channel using our quality control guidelines and data management tools, and offer recommendations for improved data yields. Our experience provides a template for other groups contemplating using SeaFET technology as well as general steps that may be helpful for the design of data management for other complex sensors.

1. Introduction

Globally, oceans are experiencing long-term change as they continue to absorb atmospheric carbon dioxide that was produced by human activities. The symptoms of this process, termed ocean acidification (OA), are a decrease in both seawater pH and the concentration of carbonate ions. OA has emerged as a major international research area emphasizing such topics as impacts on critical marine ecosystems (Doney et al., 2012), biological responses of calcifying marine organisms (Hofmann et al., 2010), and projected losses to economically valuable fisheries (Branch et al., 2013; Cooley et al., 2012). However, persistent gaps in our knowledge about the ecological impacts of OA remain, e.g., whether evolutionary adaptation is a potential response to future acidification (Kelly and Hofmann, 2012; Munday et al., 2013; Sunday et al., 2014). Insight about the potential responses of present-day marine populations to future ocean change requires knowledge about the abiotic environmental history of populations under study.

This motivation to measure pH continuously in situ has driven the development of several high-quality autonomous sensors, including

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Abbreviations: ALC, Anacapa Island Landing Cove; ARQ, Arroyo Quemado Reef; BCO-DMO, Biological and Chemical Oceanography Data Management Office; CCAN, California Current Acidification Network; Cl-ISE, chloride ion-sensitive electrode; CTD, conductivity temperature depth; DIC, dissolved inorganic carbon; DOI, Digital Object Identifier; E^*_{INT}, the Durafet® calibration constant; EML, Ecological Metadata Language; EPOCA, European Project on OCean Acidification; GOA-ON, Global Ocean Acidification Observing Network; IOOS, Integrated Ocean Observing System; ISFET, ion-sensitive field effect transistor; IWGOA, International Working Group on Ocean Acidification; LTER, Long Term Ecological Research; MBARI, Monterey Bay Aquarium Research Institute; MKO, Mohawk Reef; MCR, Moorea Coral Reef; OA, ocean acidification; OMEGAS, Ocean Margin Ecosystem Group for Acidification Studies; PUR, Purisima Point; PRZ, Santa Cruz Island Prisoner's Harbor; SBC, Santa Barbara Coastal; SBH, Santa Barbara Harbor; SMN, San Miguel Island; SIO, Scripps Institution of Oceanography; TA, total alkalinity.

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the SeaFET, which utilizes a commercially available pH electrode, the Honeywell Durafet® (Martz et al., 2010). Recent deployments of these sensors have begun to improve our understanding of natural variability in many marine systems (Frieder et al., 2012; Hofmann et al., 2011 and references therein; Kapsenberg and Hofmann, 2016; Kapsenberg et al., 2015; Krause-Jensen et al., 2015; Matson et al., 2011; Price et al., 2012; Rivest and Gouhier, 2015), with particular insights for shallow coastal oceans. pH regimes in coastal marine ecosystems differ from open ocean regimes, making high frequency, site-specific pH measurements essential for predicting biological responses to future change (Hofmann et al., 2014a). These pH measurements also provide the foundation for environmentally relevant laboratory experiments and empirical assessments of the impacts of future global ocean change on present-day populations (e.g., Frieder, 2014; Kapsenberg and Hofmann, 2014; McElhany and Shallin Busch, 2012; Rivest and Hofmann, 2014). Additionally, data from field campaigns further the general understanding of larger scale patterns of natural pH variability, facilitating multi-ecosystem and regional comparisons that identify sites of high-risk or even resilience to OA (Hofmann et al., 2014b). Such an effort requires preservation, cataloging, and distribution of several different types of pH data, with processes that are streamlined and coordinated across the OA research community.

To create pH time series that are valuable resources for the OA community, we have leveraged the U.S. Long Term Ecological Research (LTER) platform to develop careful workflow approaches. Long-term data provide a context for evaluating the nature and speed of ecological change, interpreting its effects, and predicting the range of future biological responses (Hofmann et al., 2013) - major goals of the LTER Network. Linking patterns of seawater chemistry with ecological processes across a wide range of temporal and spatial scales requires a sophisticated infrastructure of coordinated research and data management. The LTER site programs have developed such an infrastructure that can be used as a model for designing a robust strategy for generating and managing pH datasets for ecologists.

Despite the emerging importance of collecting and managing pH data, the sensors have only recently become commercially available, and the use of this technology itself is not widespread within the marine ecological community. Currently, research groups with interests in marine ecology (e.g., the LTER sites) or in ocean observing (e.g., the Integrated Ocean Observing System (IOOS); http://www.ioos.noaa.gov/) have led the collection of OA-related oceanographic datasets. A network of research-related coastal sensors is expanding on the U.S. West Coast with several groups combining sensors and assets, e.g., the Global Ocean Acidification Observing Network (GOA-ON, http://www.pmel.noaa.gov/co2/GOA-ON/; Newton et al., 2015). While ecologists, oceanographers, and organismal biologists recognize that investigators will need to converge on a set of practices for data quality management and metadata, at present, data management is self-organized, and data are available from multiple repositories. Additionally, management of OA-related datasets is a targeted goal of the U.S. Interagency Working Group on Ocean Acidification with short-term goals (3–5 years) to establish standardized measurement protocols, including for cross-agency data management and integration (IWGOA, 2014). However, to date, research and monitoring groups have not reached consensus for standardized practices for management and curation of these ocean chemistry datasets.

Here, we present a workflow “pipeline” for using DuraFET®-based pH sensor technology and incorporating appropriate data management that is presently absent from the literature. We highlight the complexities and “lessons learned” from our efforts with ongoing research in benthic coastal marine habitats. We describe our experiences with deployments and data management for SeaFETs at two coastal marine LTER sites, Santa Barbara Coastal (SBC) and Moorea Coral Reef (MCR). Deployments at both sites characterize near shore (<30 m depth) ocean chemistry. The SBC LTER focuses on a temperate kelp forest ecosystem and the MCR LTER on tropical coral reef ecology. Our first “reference” dataset for SeaFETs was developed through MCR LTER, with subsequent work focused on a SeaFET sensor network and associated data management for the Santa Barbara Channel, CA. Our association with these two LTER sites afforded two major advantages: (a) availability of data management professionals, which allowed incorporation of management practices early in the data collection process, and (b) the expectation that any deployment or data management process we developed could be applied broadly, i.e., beyond a single locale or laboratory. To help expand the use of these sensors and improve the quality and utility of pH time series data, we include a review of best practices for deployment, calibration, and data processing for Durafet®-based pH sensors, particularly the SeaFET, adding details for a variety of quality control procedures. Our experience provides insight on the investments of time and resources required for proper instrument use in an ecological context. We also present a summary of sensor performance and data recovery (73 deployments) plus a discussion of the data product design processes for several different types of pH sensor data. Our work complements curation efforts for other types of OA data within the international research community (i.e., European Project on OCean Acidification, EPOCA, http://www.epoca-project.eu). Due to the collaborative nature of utilizing LTER ocean moorings and detailed processing of SeaFET instruments and data, we have encountered most of the general issues associated with characterizing seawater pH variability in coastal environments. While SeaFETs are the focus of this work, many of the aspects of their deployment are broadly applicable to other autonomous Durafet®-based pH sensors that have become available recently (e.g., various instruments from Sea-Bird Electronics). Thus, our experience provides an effective template for other groups contemplating a similar endeavor as well as for the design of data management for other complex sensors.

2. Materials and methods

2.1. pH sensor deployment for marine ecological research

The autonomous seawater pH sensor, SeaFET, was developed and tested at Monterey Bay Aquarium Research Institute (MBARI) by Martz et al. (2010), refined at Scripps Institution of Oceanography (SIO) (Bresnahan et al., 2014), and is now commercially available from Satlantic (http://SATLANTIC.com/seafet). The ISFET technology appears to be superior to the glass electrode that plagued earlier autonomous seawater pH measurements with drift, irreproducibility, and fragility (Easley and Byrne, 2012). SeaFET sensors include an independent external chloride ion-sensitive electrode (Cl-ISE) reference and the Durafet®'s built-in internal reference electrode (Martz et al., 2010), and dual pH voltage outputs (see 2.1.6 Data processing and quality control). An embedded thermistor provides a temperature voltage.

The current state of knowledge of SeaFET deployment and calibration is summarized by Bresnahan et al. (2014), Dickson et al. (2007), Martz (2012), and Martz et al. (2010), and these combined recommendations assure the most accurate and precise data for calculations of the carbonate chemistry system. Methods described here balance the stringent requirements of the chemical oceanography community with practical field limitations of ecological investigations. We also present procedures for data processing and dataset design and management that are flexible enough to accommodate either need. Fig. 1 summarizes the general steps of a SeaFET deployment alongside the steps of data package design.

2.1.1. Deployment design

As with all moored instruments, deployment length is limited by battery life, sampling frequency, data storage, biofouling, and site accessibility. Battery life is a function of seawater temperature and sampling frequency, which is selected as appropriate for the time scale of the anticipated pH variability. Our experience in productive temperate and

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