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 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
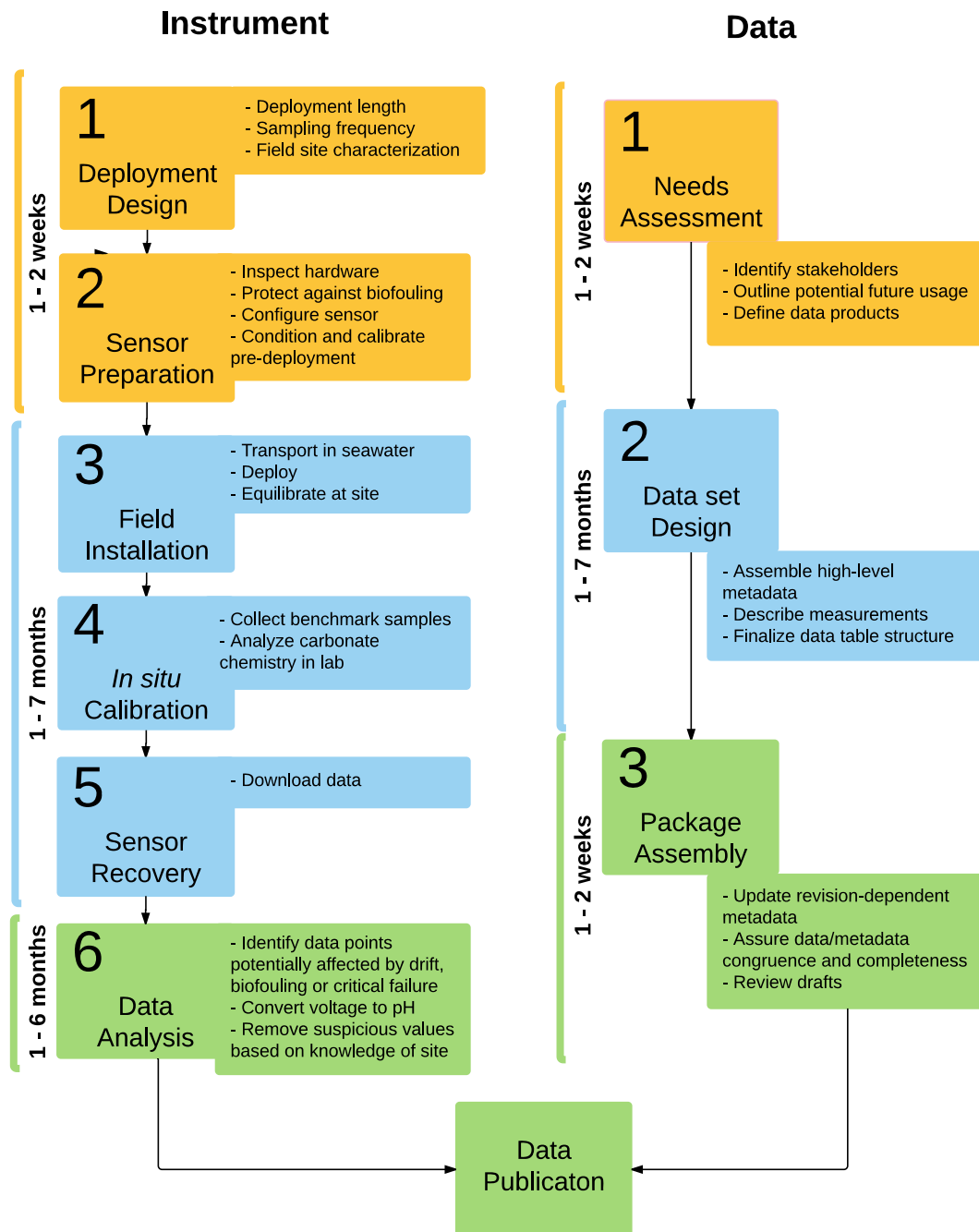
Instrument

Data

Fig. 1. Schematic workflow describing the concomitant processes for handling of autonomous pH sensors (left) and their data (right). Three major stages for each process are given (see text), with approximate durations: For instrumentation, these are Preparation (orange, steps 1, 2), Field collection (blue, steps 3–5), and Data processing (green, step 6). Three analogous phases are given for data management, also with approximate time required. Resources available for each component include a deployment checklist for users (see Supplementary Material), a guide for collecting and preserving calibration water samples (Kapsenberg, 2016), and a data processing workflow (see Supplementary Material).

tropical coastal marine environments suggests that constraints can be balanced with 10- or 20-min sampling frequencies and 1–3 month deployments (Fig. 1). In regions with low biofouling (e.g. coastal Antarctica), we have successfully collected data for up to 7 months, limited by battery power (Kapsenberg et al., 2015).

Autonomous pH sensors have been successfully used in many habitats (Hofmann et al., 2011) using various infrastructures. Stainless steel mesh and protective perforated PVC housing for intertidal habitats, and anchored stainless-steel posts allow the SeaFET to be secured for benthic deployments on rocky substrates in wave-swept environments. Hose clamps are used to attach SeaFETs to any cylindrical feature – pier pilings, subtidal pipes, etc., and mid-water deployments use a traditional mooring cage.

2.1.2. Sensor preparation

For each deployment, several preparatory steps help to ensure that reliable, high-quality data are collected: (1) hardware inspection, (2) protection of the sensor from biofouling, (3) sensor configuration, (4) conditioning in seawater, and (5) laboratory calibration (following Bresnahan et al., 2014). In our experience, sensor preparation takes approximately one week, as dry electrodes require soaking time to condition.

2.1.2.1. Hardware inspection.
We verify battery condition, look for physical damage to the surface of the sensing chips of both electrodes, and ensure that sealing surfaces of the housing are intact (no dust or

scratches that might break the seal). Damaged electrodes typically cannot be repaired and must be replaced.

2.1.2.2. Protection against biofouling. Preventing the SeaFET from encrustation by settling organisms is essential because their respiration and photosynthesis alters pH of the immediate chemical environment. We typically employ five mechanisms to prevent data loss due to biofouling: before deployment, 1) wrapping instrument housing with electrical tape, 2) antifouling paint for housing, 3) copper mesh housing for electrode surface, followed by 4) regular cleaning during deployment and/ or 5) photographic documentation at sensor recovery. Additionally, actively-pumped sensors typically delay the onset of fouling compared to non-pumped sensors like the SeaFET (Bresnahan et al., 2014). In a temperate sea grass bed, biofouling still occurs within three months, while in near-shore Antarctica, sensors can exhibit little fouling for up to one year (Fig. 2). With routine cleaning during deployment, fouled sensors usually return to recording accurate pH values within hours (Bresnahan et al., 2014). Photographic documentation upon instrument recovery records condition to help with data interpretation later.

2.1.2.3. Configuration. Routine configuration (sampling interval and signal averaging) should also include clock synchronization to a referenced time to ensure an accurate match with timing of collection of benchmark samples.

2.1.2.4. Conditioning. The sensor should be submersed in seawater for a minimum of 7–10 days prior to deployment (Bresnahan et al., 2014) to allow the Durafet® and Cl-ISE electrodes to equilibrate. The need for a pre-conditioning period is well-documented (Bresnahan et al., 2014), and careful planning prevents loss of data early in the time series.

2.1.2.5. Pre-calibration. Current best practices state that the sensor should be calibrated in the laboratory between conditioning and deployment ('shore-side calibration' or 'pre-calibration,' Bresnahan et al., 2014). Ideally, during pre-calibration, the sensor is operated continuously in seawater under known temperature and salinity conditions,

with multiple discrete bottle samples collected across a range of seawater pH. Alternatively, sensor performance and drift can be assessed across a range of temperatures using a known standard, such as Tris buffer (also see 2.1.6 Data processing and quality control or Bresnahan et al., 2014). We have found that for our ecological parameterizations, if a calibration facility is not available, an in situ calibration can be substituted (discussed below, 2.1.4 In situ calibration and benchmark samples).

2.1.3. Field deployment

En route to the deployment site, the sensor electrodes must be kept immersed in seawater to ensure high-quality data collection immediately upon deployment. At the field site, we orient the SeaFET with electrodes facing down to minimize sedimentation on the sensing surfaces and protect them from large debris. We have found that the watertight seal of the cylindrical housing can be compromised by over-tightening hose clamps or other fasteners, so at permanent sites (e.g., pilings), we use a PVC mounting frame fitting the curvature of the housing. Although the electrodes have been equilibrated to seawater prior to deployment, an equilibration period following deployment frequently occurs due to field conditions of salinity and temperature.

2.1.4. In situ calibration and benchmark samples

Our experience indicates that in lieu of a pre-calibration, an in situ calibration can be accomplished by collecting multiple field seawater samples close in time and space to the sensor as it records data, hereafter referred to as a "benchmark" samples. Laboratory measurements of pH, total alkalinity, and salinity from benchmark samples confirm in situ conditions of carbonate chemistry over the entire deployment. These physical seawater samples are the most direct measurements of seawater chemistry at the study site (Riebesell et al., 2010), and the autonomous sensor data simply fill the gaps. So, for the best possible calibration of sensor data, it is important to take as many in situ benchmark samples as is practical.

Our collection and analysis of all discrete water samples follows the guidelines described by Dickson et al. (2007). Ideally, the benchmark
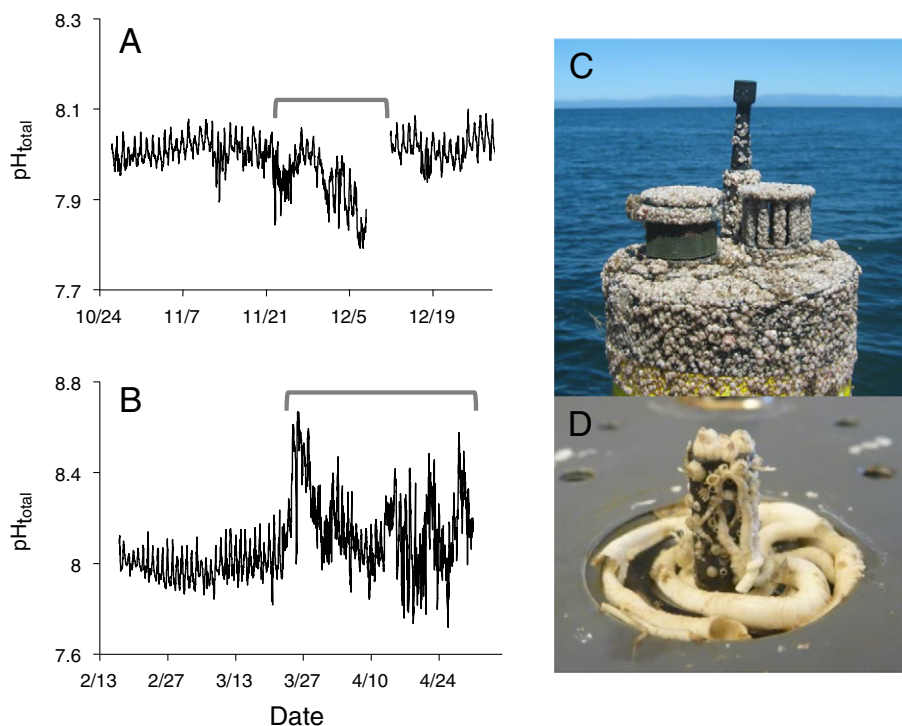

Fig. 2. A–B. Two examples of biofouling events (gray brackets) occurring near the end of deployments on a piling. C–D. Extreme fouling on electrodes that were not sufficiently protected by copper caps or mesh.

samples represent the same water that the sensor is measuring. Because pH may vary substantially over small spatial and temporal scales in coastal systems (Frieder et al., 2012), careful attention must be paid to the precise timing and location of sample collection. If these do not *exactly* coincide with the sensor data collection, then the sensor voltages are interpolated to the exact time stamp of the bottle sample. We have found that the most reliable method for collecting benchmark samples is by a SCUBA diver with a Niskin bottle. If the instrument is shallow enough to be visible from the ocean surface, samples can be taken by hand or using a cabled Niskin and messenger.

Benchmark samples are returned to the laboratory for analysis. Calculation of temperature-corrected in situ pH plus associated carbonate chemistry parameters (e.g. partial pressure of CO_2, aragonite saturation state, etc.) requires measurements of at least two parameters of seawater carbonate chemistry, temperature, salinity, depth, and nutrients (e.g. phosphate, nitrate, silicate). Several approaches are possible for measurements of the carbonate system (e.g. dissolved inorganic carbon (DIC), pCO_2); data presented here used direct measurements of pH and total alkalinity (TA). Seawater pH in benchmark samples was measured spectrophotometrically following Dickson et al. (2007, SOP 6b). We have found that commercially available, unpurified m-cresol purple dye (Sigma-Aldrich®) produces a pH offset of -0.02 to -0.04 (-0.032 ± 0.006) among individual operators (Kapsenberg et al., 2015), estimated by comparing pH measurements of reference materials (courtesy of Dr. A. Dickson, batch 108) to values calculated from their DIC and TA certification. If purified m-cresol dye becomes commercially available, our accuracy is expected to improve by nearly 0.02 units (Liu et al., 2011). TA was measured by potentiometric titration with 0.1 N HCl in 0.6 M NaCl on a Mettler-Toledo T50 automatic titrator (Dickson et al., 2007), and salinity from benchmark samples using a benchtop digital meter (YSI 3100 Conductivity) or from a calibrated CTD that was deployed simultaneously with the SeaFET. With these inputs alongside spectrophotometric pH and environmental temperature, pH at in situ conditions plus the full suite of carbonate system parameters is calculated using CO2CALC (Robbins et al., 2010).

2.1.5. Sensor recovery

After a sensor is recovered, it can be transported wet or dry and while recording, so generally, we delay data download until reaching the laboratory. Raw data download varies by sensor type; SIO SeaFETs export timestamp, battery voltage, temperature, internal electrode voltage (Durafet®), and external electrode voltage (Cl-ISE). Satlantic SeaFETs export factory-calibrated pH and temperature directly, but raw voltages can obtained through SeaFETCom.

2.1.6. Data processing and quality control

The strategy for processing data differs slightly depending on the calibration scenario. In order of preference, these are: (1) numerous benchmark samples collected throughout a deployment, (2) 2–3 benchmark samples, and (3) a single benchmark sample. Quality control procedures will help to distinguish true pH variability from signals caused by poor sensor conditioning, biofouling, and electronic failure. Particularly, an understanding of sensor behavior and local pH variability are essential for identifying suspicious pH values (described below). It is important to note that one's ability to assess the quality of the data is ultimately limited by the number and quality of benchmark samples collected during the deployment, as well as the use of simple pre- and post-deployment calibrations. However, collection of one to a few benchmark samples may be adequate for studies of pH variability on shorter timescales or during episodic events.

2.1.6.1. Screening. Initial processing removes sensor data collected during periods of conditioning, drift, and failure. First, the time series is trimmed to exclude the conditioning period following field deployment (hours to weeks, Bresnahan et al., 2014). Next, measurements with raw voltages outside an acceptable range are flagged as suspicious. Expected

ranges for SeaFET electrodes in seawater are 0.04 to 0.1 V for the internal reference electrode (Durafet®) and from -0.9 to -0.85 V for the external reference electrode (Bresnahan et al., 2014; Martz, 2012). However, it is very important for users to understand sensor behavior at their study sites and to compare deployment data with regularly collected bottle samples to gauge the expected raw voltage range of a specific sensor.

Comparisons of the voltage data from the internal (Durafet®) and external (Cl-ISE) electrodes may be used to identify periods of conditioning, the onset of biofouling, and sensor failure. Presently, we are most concerned with identifying these sources of poor-quality data because while drift can occur due to problems with an electrode's electrolyte gel or liquid junction, its data anomalies are often an order of magnitude smaller than anomalies due to biofouling and critical failure (Bresnahan et al., 2014). For the LTER workflow, data are flagged as suspicious if the difference between internal electrode pH and external electrode pH $> |0.04|$. The external reference electrode is more sensitive to changes in salinity than the internal electrode, so the tolerance window may be site-specific. However, the electrode voltage comparison is only one metric for determining overall SeaFET performance, and eliminating data based on voltage comparison alone may yield smaller datasets that are not necessarily higher in quality. The internal reference electrode (primary source for pH data) may continue to function normally when the external reference electrode fails, and either the internal or external electrode can be used to generate a high-quality pH dataset (Martz et al., 2010). We also recommend against using the internal-external comparisons to strictly identify onset of biofouling in the absence of other (visual) indicators.

2.1.6.2. Converting raw sensor voltage to in situ pH. The final in situ pH dataset is generated using voltage data from the internal Durafet® pH electrode, due to the lack of salinity dependence of the electrode in the range of 30–36 PSU when using the total hydrogen ion scale (the accepted pH scale for ocean carbonate chemistry data; Bresnahan et al., 2014). In the event that this electrode fails, the pH dataset may be recovered through use of the external (Cl-ISE reference) electrode. Because the external electrode is roughly $100\times$ more sensitive to salinity than the internal electrode (Martz et al., 2010), concurrent salinity time series are necessary in this scenario.

Seawater pH is calculated from sensor voltages using the calibration constant, E^*_{INT}, an offset calculated as the regression intercept of benchmark sample pH against sensor pH, such as those from pre-deployment calibration (Bresnahan et al., 2014). When a pre-deployment calibration was not performed, E^*_{INT} can be calculated from field-collected benchmark samples with one of three scenarios, depending on the number of benchmark samples collected during the deployment (many, few, or one). However, only benchmark samples collected after field equilibration and before the onset of biofouling can be used to calculate E^*_{INT}. For all data sets, it is appropriate to report all available calibration and benchmark sample data along with the pH time series.

When many (>10) benchmark samples have been collected during a deployment (the ideal scenario), E^*_{INT} can be calculated for the entire time series using the same regression method as is used for pre-deployment calibration samples (Equation 5, Bresnahan et al., 2014). Our sites have limited access, and typically only 2 or 3 reliable benchmark samples are available per deployment. In this case, E^*_{INT} is calculated by minimizing the difference between benchmark sample pH and sensor pH. Having only a few benchmark samples means that the effect of spatiotemporal mismatch of any one sample on the entire time series will be greater, and ideally, such datasets should report the site-specific spatio-temporal sampling error (e.g., Bresnahan et al., 2014; Kapsenberg and Hofmann, 2016). We are adding this information to the LTER workflow. When only one benchmark sample is collected, its pH and the corresponding sensor voltage are used to calculate E^*_{INT}. While acceptable, the application of E^*_{INT} from a single benchmark sample limits the assessment of biofouling or sensor failure.

The pH time series can then be used to calculate other carbonate system parameters (e.g., pCO$_2$, saturation states). We use mean total alkalinity (TA) from benchmark samples as the second carbonate chemistry parameter. If conductivity/temperature/depth sensor (CTD) data are available, the TA time series can be estimated using existing relationships of temperature and salinity (e.g., as done in Kapsenberg and Hofmann, 2016). However, empirical temperature-salinity-TA relationships established for open ocean regions (Lee et al., 2006) present limitations in marginal seas and highly variable coastal environments where external sources of high alkalinity (e.g., rivers (Raymond and Cole, 2003), submarine groundwater springs (Cai et al., 2003)) alter these algorithms. We recommend that users fully describe the limitations and propagated errors in pCO$_2$ and saturation states derived from SeaFET pH data.

2.1.6.3. Site-specific quality control. Following the initial inspection of voltage data and conversion to seawater pH values, data points are flagged and evaluated based on knowledge of pH variability in the respective deployment sites. For example, our southern California coastal rocky reef kelp forest sites typically experience wide pH variability, and we flag pH values that are outside the range of 7.5–8.5 and whose residuals from a six-hour low pass filter exceed |0.045| (indicating that pH is changing faster than expected in situ). These parameters are based on our site-specific corpus of SeaFET data and provide an automated way to identify affected values, e.g., by instrument failure or biofouling. Users should determine appropriate ranges for their own study sites. All flagged values should be considered individually before exclusion from downstream analyses, using experiential knowledge of local environmental variability. Values that fall within the site-specific pattern of variability are categorized as 'good quality' and those outside that range as 'suspicious.' For the purposes of this workflow, 'good data' are considered to be all data not flagged and that represent perfect simultaneous functioning of both the internal and external electrodes in the SeaFET.

2.1.6.4. Biofouling. In general, it is recommended to eliminate data where biofouling can be identified (i.e., through the use of time series anomaly plots and multiple benchmark samples; Bresnahan et al., 2014). Biofouling can be identified as unusual pH patterns, such as drift, a sudden steady decline in pH, extremely high diurnal variability, or poor congruence with the pH of benchmark samples or a consecutive sensor deployment (Fig. 2A,B). At SBC sites, biofouling often produces a negative pH anomaly, presumably due to localized respiration or calcification; however, positive anomalies could be generated through an increase in net photosynthesis (which could be corroborated by the presence of a phytoplankton bloom) or CaCO$_3$ dissolution (Fig. 2B). With many ($n \geq 10$) benchmark samples plus visual observations of the sensor, users can more accurately identify drift in pH due to biofouling (Bresnahan et al., 2014). With few calibration samples, the timing is difficult to ascertain. Elimination of ostensibly bad data is recommended, as once fouling is capable of affecting sensor pH, the resulting values are not representative of the bulk seawater environment.

2.2. SeaFETs (autonomous pH sensors) as a use case for planning and design of data sets

We employed the sophisticated data management system of two sites of the U.S. LTER program (SBC and MCR; http://sbc.lternet.edu and http://mcr.lternet.edu, respectively), leveraging their experience with metadata specifications, data curation, long-term preservation, Digital Object Identifiers (DOIs), and delivery through federated systems. LTER sites emphasize the packaging of data for effective reuse.

Data management activities (Fig. 1, right) were carried out concomitantly with the development of SeaFET deployment and data processing strategies, with contributions from research laboratories working in multiple coastal areas and based at the University of California, Santa Barbara. Consideration of the need for data publication early in the planning process has several benefits. First, planning for data storage maximizes security and minimizes the risk of future loss. Second, planning for eventual dissemination of data products requires a data curator to be involved, bringing an independent point of view from someone well versed in a wide variety of data types and processing issues. Discussions of data description provide a venue for continuous assessment of methods and enable more rigorous quality analyses. Collaboration between data curators and scientists ensures that data products adhere to both the current recommendations for the highest quality of data description from the informatics community and also to those of scientific communities such as EPOCA and California Current Acidification Network (CCAN; http://c-can.msi.ucsb.edu/). Our documentation of the data set design process itself provides a template for data from other areas of research.

2.2.1. Needs assessment

We established the initial parameters for SeaFET data management through existing LTER Network venues and processes and assembled a working group of scientists and data managers to advise on high-level considerations. Discussions generated recommendations for text fields (e.g., abstracts, labels), approved keyword vocabularies, guidelines for refining measurement descriptions, as well as more complex considerations such as the differentiation between data resulting from passive, in situ observations and those from process studies or manipulations (Gastil-Buhl et al., 2012). Consultation with other researchers with similar projects (i.e., EPOCA) helped us align our efforts with complementary data management for other types of OA research.

2.2.2. Dataset design

We anticipated data from both short-term process studies and long-term ongoing time series, with all products appropriate for long-term archival in a data repository. A process study of pH, temperature, and associated carbonate chemistry on a fringing coral reef in Moorea, French Polynesia provided a reference SeaFET data set (Rivest and Hofmann, 2012). We further refined those measurement descriptions to develop several distinct data products and generalized them for reuse in both SeaFET time series and in process studies. As with all data sets developed by the SBC and MCR LTER sites, metadata was maintained in a relational database system, exported per the XML specification Ecological Metadata Language (EML, Fegraus et al., 2005), and drafts of data set templates were available online for review by scientists.

2.2.3. Data package assembly

Data packages (data tables and EML metadata) were assembled using appropriate pathways established for other SBC LTER data (O'Brien, 2015). SeaFET time series data were expected to employ a template, with data from multiple instruments or sites produced quickly and in the same format in series, whereas a data package for benchmark samples was expected to be unique. When data tables included the suite of carbonate chemistry parameters calculated from pH data (i.e., binned time series and benchmark samples design patterns, see below), we used the same format as the CO2CALC program (Robbins et al., 2010). These data table templates include columns for all possible inputs for the calculations; input data are clearly labeled, with missing values coded. While users could easily produce the suite of CO2CALC outputs on their own, we include it for ease of reuse and for comparison. As the last step, analysis personnel construct the EML metadata records from templates as the last step in data processing using Matlab. All datasets and metadata are deposited in the LTER data catalog and the metadata consequently harvested by aggregators (e.g., DataONE.org).

3. Results and discussion

Since 2011, we have conducted 73 SeaFET deployments throughout the Santa Barbara Channel (Table 1). Insights gained from these SeaFET data have contributed to the understanding of natural temporal and

Table 1

Description of all SBC LTER SeaFET deployments to date, with summarized data characteristics. When an in situ calibration of SeaFET data using benchmark samples was possible, it is indicated. The number of benchmark samples collected during each deployment is stated in parentheses. No deployments had laboratory calibrations. The equilibration period following deployment was determined by the difference between the Durafet® and Cl-ISE electrode voltages. Periods of critical failure, where sensor voltages fluctuated wildly, quickly trended out of acceptable range) with no underlying pattern, or signal, or flat-lined, included battery issues and/or faulty electrodes and typically lasted for the remainder of the deployment. Suspicious data, including evidence of biofouling (marked with *), are based on the numerical criteria described in 2.1.6 Data processing and quality control, and also by experiential knowledge of natural pH variability at each site. Blank cells indicated 0%. Site abbreviations: ALC – Anacapa Island Landing Cove, ARQ – Arroyo Quemado Reef, MKO – Mohawk Reef, PUR – Purisima Point, PRZ – Santa Cruz Island Prisoner's Harbor, SBH – Santa Barbara Harbor, SMN – San Miguel Island (see http://sbc.lternet.edu for more details).

Sensor ID	Deployment site	Start date	Length (days)	In situ calibration? (benchmark samples)	Percent of time during deployment with data characteristics:			
					Field equilibration	Critical failure	Suspicious	Good quality
18	MKO	7/20/11 23:37	90.84	N (0)			100%	
18	MKO	1/11/12 1:03	86.67	Y (1)	1%		35%	65%
18	ALC	12/13/12 0:23	145.54	Y (1)	4%	15%	27%	54%
18	ALC	8/7/13 17:56	99.01	Y (1)				100%
18	SMN	1/16/14 16:46	66.97	Y (3)				100%
18	ALC	4/24/14 19:38	61.84	Y (2)	8%			92%
18	MKO	1/7/15 20:33	30.02	Y (4)				100%
19	MKO	10/20/11 1:37	81.04	N (0)	1%	90%		9%
19	ALC	9/4/12 17:20	95.30	Y (2)	5%	34%	43%	19%
19	SMN	8/19/13 18:07	72.97	Y (2)				100%
19	ALC	11/14/13 16:13	83.10	Y (5)				100%
19	SMN	3/24/14 20:52	76.83	Y (1)				100%
19	ALC	6/26/14 1:15	86.73	Y (2)				100%
19	ALC	12/19/14 23:16	80.95	Y (1)	12%			88%
19	MKO	5/14/15 1:29	26.67	N (1)				100%
20	ARQ	9/12/14 19:51	28.02	Y (2)	43%		57%	
20	MKO	11/4/14 21:15	27.82	Y (1)		100%		
32	ALC	5/13/13 1:10	86.81	Y (2)				100%
33	PRZ	5/19/13 23:04	76.89	Y (2)				100%
36	ALC	2/18/12 19:14	87.75	Y (2)	6%			95%
36	SMN	10/31/13 16:02	77.02	Y (1)				100%
36	ALC	2/5/14 20:59	77.94	Y (3)	1%			99%
36	SMN	6/9/14 15:33	72.60	Y (1)	16%			84%
36	ALC	9/21/14 2:32	107.17	Y (1)		100%		
37	PRZ	2/18/12 1:50	87.84	Y (1)				100%
37	PRZ	9/4/12 21:54	93.80	Y (1)				100%
37	ARQ	10/12/12 16:28	97.13	Y (2)				100%
37	PRZ	12/12/12 13:22	158.01	Y (1)			35%	63%
37	ARQ	10/4/13 17:26	95.87	Y (5)	4%			95%
37	MKO	2/11/14 21:03	97.00	Y (7)	4%		67%	29%
37	MKO	7/2/14 22:00	29.73	Y (1)		64%		36%
37	ARQ	12/5/14 21:03	31.89	N (0)				100%
37	SBH	2/2/15 17:40	85.89	Y (2)				100%
37	PRZ	5/4/15 20:41	79.84	N (1)				100%
39	MKO	4/6/12 16:05	102.04	Y (2)	12%			89%
39	MKO	1/29/13 17:38	93.04	Y (2)		100%		
39	ARQ	4/10/14 16:01	89.17	Y (4)	5%			95%
39	ARQ	8/14/14 19:45	28.97	Y (1)				100%
39	MKO	10/13/14 18:59	22.02	Y (1)			100%	
39	ARQ	11/13/14 18:51	21.69	N (2)			59%	40%
39	ARQ	1/6/15 20:07	27.06	Y (1)			45%	55%
42	MKO	7/17/12 16:48	97.15	Y (1)	12%			87%
42	SBH	12/7/12 18:34	119.03	Y (15)		71%		28%
42	ARQ	4/10/13 18:20	90.88	Y (4)	7%			92%
42	SBH	3/21/14 13:47	102.98	N (0)				100%
42	MKO	8/1/14 22:35	38.90	Y (2)				100%
42	ARQ	10/10/14 18:59	34.02	Y (2)		19%		81%
43	MKO	4/6/12 16:05	102.04	Y (2)	19%			81%
43	SBH	9/14/12 17:29	83.97	Y (12)	1%	72%		27%
43	SBH	10/1/13 23:35	76.92	Y (7)				100%
43	ARQ	1/8/14 21:39	91.93	Y (2)				100%
43	MKO	5/20/14 3:45	43.41	Y (4)	7%			94%
43	ARQ	7/8/14 17:28	37.10	Y (1)	15%			84%
43	MKO	9/9/14 21:59	33.93	Y (2)		12%	54%	34%
43	SBH	10/24/14 18:37	101.04	Y (1)	8%			92%
43	MKO	2/6/15 21:57	30.92	Y (2)			16%	83%
43	MKO	4/9/15 0:33	35.64	N (1)				100%
48	ARQ	7/25/12 16:27	79.04	Y (1)	6%			94%
48	MKO	10/22/12 21:23	74.75	N (0)	3%			97%
48	SBH	7/5/13 3:24	133.32	Y (9)		94%		6%
48	SBH	12/18/13 21:33	93.15	Y (6)				100%
48	PRZ	5/21/14 5:11	96.29	Y (6)	11%	60%		28%
48	MKO	11/26/14 17:50	42.09	Y (6)				100%
48	ARQ	2/3/15 0:17	31.81	Y (1)				100%
48	ARQ	4/6/15 23:52	35.71	N (3)		100%		
50	SBH	4/5/13 19:00	87.96	Y (11)	5%			94%
50	MKO	11/5/13 20:27	98.09	Y (5)		100%		

Table 1 (*continued*)

Sensor ID	Deployment site	Start date	Length (days)	In situ calibration? (benchmark samples)	Percent of time during deployment with data characteristics:			
					Field equilibration	Critical failure	Suspicious	Good quality
50	SBH	7/2/14 17:29	114.13	Y (1)			45%	54%
50	PRZ	11/22/14 0:29	94.50	N (1)	21%			79%
50	MKO	3/9/15 23:00	29.88	Y (3)			9%	91%
50	ARQ	5/12/15 20:39	22.88	N (1)				100%
62	PRZ	8/22/14 10:17	91.33	Y (2)				100%
62	PUR	1/7/15 22:33	62.87	Y (1)				100%

spatial pH dynamics, biological feedbacks to pH regimes, and correlations between pH and other environmental stressors in coastal ecosystems (Booth et al., 2012; Frieder et al., 2012; Kapsenberg and Hofmann, 2016)(Booth et al., 2012; Frieder et al., 2012; Kapsenberg and Hofmann, 2016). Here, we present a summary of sensor performance and data recovery and describe the role of data management to facilitate archival and sharing of these environmental data.

3.1. Sensor behavior

To date, we have recovered data from 13 SeaFETs during 73 individual deployments at 7 sites throughout the Santa Barbara Channel along with 263 benchmark samples (summarized in Table 1). Deployments had an average duration of ~70 days, and data were calibrated and processed according to Section 2. For 11% of deployments ($N = 8$), no data could be used because these instruments experienced critical failure, identified as periods where sensor voltages (Durafet®, Cl-ISE, or both) flat-lined, fluctuated wildly and rapidly or quickly trended to values out of the acceptable range with no underlying pattern or signal. Sensors rarely recovered after critical failure. In the remaining 65 deployments, 85% of data points collected were determined to be of high quality (per Section 2.1.6). Poor quality data (15%) were generally due to three sources: the electrodes were not fully equilibrated in situ at the start of the deployment, or if equilibrated, the electrodes exhibited occasional irregular behavior or biofouling.

Observations of occasional irregular behavior of Durafet® electrodes highlights the importance of collecting multiple benchmark samples throughout each deployment. Obviously, a single benchmark sample that coincides with irregular sensor behavior means that the sensor cannot be calibrated and therefore collected no useable data. This was the case in 16% of SBC deployments (Table 1). While no useable in situ pH values can be retrieved for these datasets, overall sensor performance can still be assessed, which is included in Table 1.

Overall, an individual SeaFET performed well 70–80% of the time (Table 1). We retrieved good quality data for ~74% of each deployment (SD = 26%). A single instrument exhibited critical failure in ~21% of its deployments, with no pattern of failure among instruments. We expect an improvement in future data yields, as both instrument performance and our proficiency improve.

Data processing and quality control procedures continue to evolve. Site-specific variability in pH means that data evaluation is time consuming and still somewhat subjective. As our understanding of local regimes improves, parameters can be tuned to produce more objective measures of data quality. Pre-deployment laboratory calibrations and increased numbers of benchmark samples will minimize data gaps and improve the fit of calibration coefficients. Finally, as global change ecologists, we strive to balance the tradeoff between ideal sensor operation and data that is fit-for-purpose. Users need to find the right balance of allocation of resources between those needed for sensor deployments, calibration and sample analysis, and data management with those needed for co-located hypothesis-driven ecological studies.

3.2. Data management

In developing appropriate data products for our sensor data, we borrowed a term from software engineering - "design pattern", a repeatable solution to a recurring task (e.g., Pressman, 2005). Design patterns serve as templates, are improved over time, and become widely understood, making them more robust than ad-hoc designs. Our work has led to the development of three distinct design patterns suitable for both short-term process studies and for ongoing time series (Table 2). Each pattern underscores a unique benefit of data management and use of autonomous pH sensors for contextualizing ecological OA research. Together, this suite provides wide coverage of carbonate features for a variety of uses.

The first design pattern, "single deployment," is composed of calibrated data from an individual SeaFET deployment at the original sampling frequency (Table 2, Fig. 3A), conceptually similar to the Level 1 data product defined for NASA instrument data (NASA, 2010). It includes appropriate ancillary information (e.g., voltages, temperature, salinity, pH at time of calibration, calibration method), processed using the calibration and quality control techniques described in Section 2. With this pattern, data at the original sampling frequency are provided for users applying alternative quality control procedures or for ingestion by workflow code assembling longer time series from individual deployments. It also serves as a deployment archive. Single deployments may stand alone or accompany biological experimental data and peer-reviewed publications, e.g., where time series pH data provide ecological context for the experiments.

The second pattern, "binned time series" (Table 2, Fig. 3A,B) contains quality-controlled values of calibrated SeaFET data (including the entire suite of calculated carbonate chemistry variables), resampled and interpolated at a time interval compatible with other LTER data products from co-deployed sensors (e.g., CTD, ADCP, Hofmann and Washburn, 2015; Fig. 3A) and is similar to NASA Level 2 derived data (2010). Use of this design pattern expedites the process of producing data sets that conform to LTER data management practices, in reliable, stable formats that can be integrated with other moored data, and amenable to future data additions.

The third pattern is for laboratory-processed data from benchmark seawater samples collected near deployed SeaFETs throughout all deployments (Hofmann et al., 2014a, Table 2, Fig. 3C). Like the binned time series, this data set includes the entire suite of carbonate chemistry parameters calculated from the measured parameters using CO2CALC. The design pattern accommodates different laboratory practices, e.g., the choice of different input variables for the calculation of the carbonate suite. This pattern is designed to be a continuous, ongoing time series of discrete samples, with new data combined with existing data.

The process for developing these three design patterns required considerable experience with SeaFET deployment, handling, and processing. The first dataset to be curated was collected ad hoc in Moorea, French Polynesia on a coral fringing reef to elucidate natural conditions experienced by coral during brooding and larval release and to establish a baseline environmental regime for a study assessing the effects of OA and warming on coral larvae (Rivest and Hofmann, 2014). SeaFET data

Table 2
SeaFET-related pH data package design patterns. "Data source" will be either from SeaFET sensors or benchmark samples analyzed in the laboratory. "Justification" gives the reason for creating the data package. "Updates expected" refers to whether data products of this type are expected to receive data additions. A "data package" is defined as an EML metadata record plus data table (see text). Features are summarized in the last column.

Name	Data source	Justification	Updates expected	Data package features
Single deployment	SeaFET sensors at SBC LTER moorings	Archive of high-frequency records (Level 1 data product)	No	One package per deployment, total number of packages indeterminate Computed values at original time resolution, scientific units Field calibration included and applied Processing intermediate (in workflow for Binned time series) Creation via Matlab with XML template, per SBC LTER practices (see text) Need for including CO2CALC output to be determined
Binned time series	SeaFET sensors at SBC LTER moorings	Core SBC LTER moored time series product (Level 2 data product)	Yes	One package per site, location in metadata Field calibration included and applied with values resampled to match time interval of other moored data at the same site Creation via Matlab with XML template, per SBC LTER practices (see text) Include CO2CALC output
Benchmark samples	Intermittent water samples, with laboratory analysis	Benchmark samples for calibration	Yes	Single unique package Multiple sites, with locations in metadata Originated and owned by multiple collaborative projects One data table, resembles laboratory spreadsheet Includes CO2CALC output

ranged from pH 8.02–8.13 and provided context for the laboratory control treatment (pH = 8.00), with treatment exposures shown to exceed environmental pH (pH = 7.73; Fig. 4). Per MCR LTER policies, these data received full archival treatment (i.e., quality controlled metadata and full congruence per O'Brien et al., 2016–in this issue), but did not require the regularized measurement descriptions of our long-term time series. These data then became a reference dataset for local standardization of measurement metadata and data table structure, and these early investments allowed us to more quickly build a data management scheme for more complex long-term deployments.

The regularized measurements found in the final design patterns reflect the lessons learned with the reference dataset. Our established high-frequency time series are planned to provide a long-term record of ocean conditions across a range of temporal scales to link pH to ecological processes and targeted biological studies. Ongoing global ocean change is predicted to perturb marine environments on a variety of time scales, e.g., extreme events on the scale of days, seasonal changes on scales of weeks to months, and climate state oscillations lasting years to decades (IPCC, 2013). The SBC LTER program has maintained moored sensors near a kelp forest at Mohawk Reef (MKO) since 2005, adding SeaFET sensors in 2011. This long-term time series reveals dynamic pH variability on multiple temporal scales (Fig. 3A), with average daily pH variability spanning ± 0.05, and lower and higher frequency oscillations caused by seasonal and annual cycles.

Table 3 describes the features, status, and final products of the current suite of SBC LTER OA-related data packages, which includes both ongoing time series and short-term process studies. Included are the original reference datasets from the Moorea study, the four binned time series regularly maintained by SBC LTER, two time series of water samples (a core ongoing time-series and a short-term study still at the
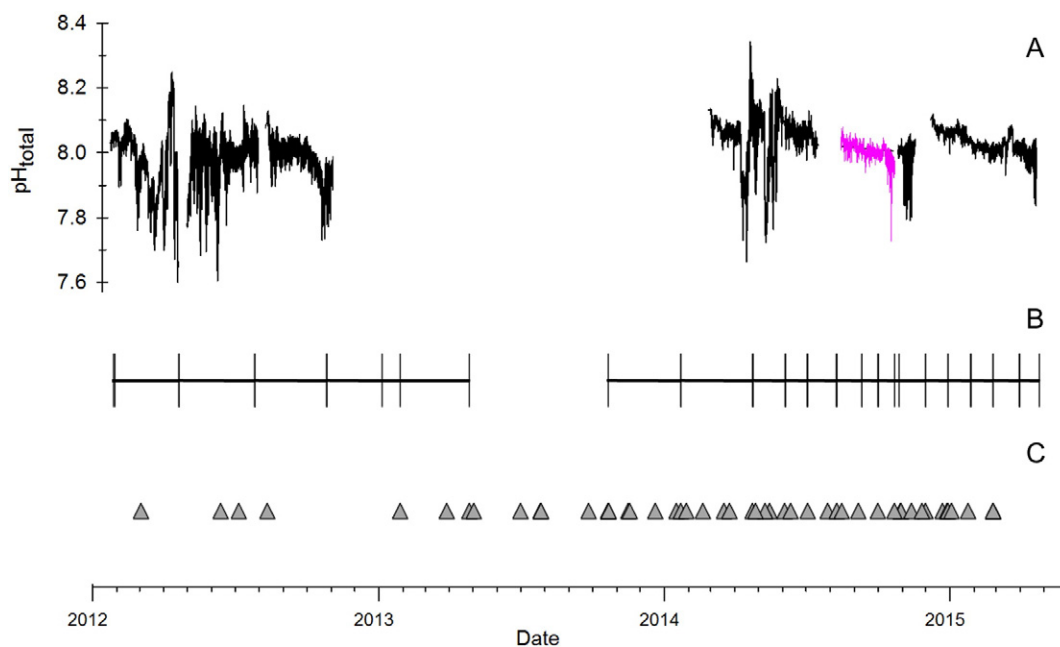

Fig. 3. Sample SeaFET data from SBC LTER showing temporal coverage for three design patterns. (A) pH time series data collected at Mohawk Reef (MKO). The 'single deployment' design pattern contains calibrated data from one deployment in one data package (for example, the one highlighted with a pink line). Calibrated data from all deployments from MKO are managed as a time series using the 'binned time series' pattern (black line). (B) Temporal coverage of the processed time series with vertical lines marking the start and end points of individual deployments. Gaps indicate intervals between deployments. (C) Timing of benchmark samples for calibration of single deployments at MKO. These samples for MKO are included with those from all other sites in the 'benchmark samples' pattern.
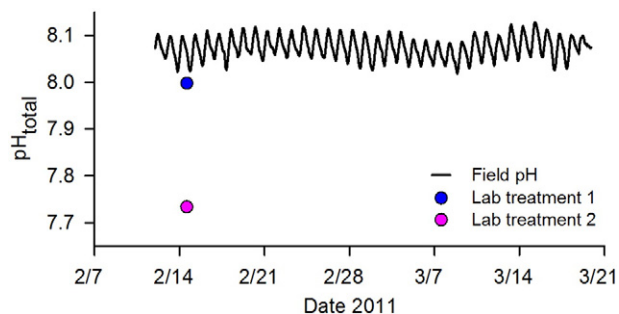
Fig. 4. pH time series data used to inform laboratory OA experiments. A SeaFET pH time series (black line) at the species' collection site for physiological studies in a tropical coral reef in Moorea, French Polynesia (Rivest and Hofmann, 2014). In the laboratory, CO_2-manipulation experiments were used to control seawater pH at values that matched present-day environmental conditions (blue circles) as well as site-specific future OA scenarios (pink circles).

design stage). Several examples of process studies that use the single deployment pattern are also included, and to date, these three design patterns have covered all our needs.

4. Future perspectives

The purpose of scientific data management is the facilitation of scientific discovery. Insights gained from SeaFET data have advanced our understanding of natural temporal and spatial pH dynamics, biological feedbacks to pH regimes, and correlations between pH and other environmental stressors (Booth et al., 2012; Frieder et al., 2012; Kapsenberg and Hofmann, 2016), illustrating the importance of biological processes (e.g., primary production) on the pH regime in an ecosystem and facilitating investigations of the next generation of biological questions. In 2015, researchers at SBC LTER deployed SeaFETs with O_2 sensors, called SeapHOxes (Todd Martz, SIO, commercially available through Sea-Bird Electronics), to characterize changes in pH and dissolved oxygen inside and outside a kelp forest during seasonal upwelling (Fig. 5). Diel changes were greater inside the kelp forest until an upwelling event apparently diminished high-frequency variability. The importance of specific pH regimes, induced by habitat forming species, in relation to ecological changes predicted by ocean change

remains unexplored. Understanding the relationship between pH regimes, patchiness, stress tolerance, local adaptation, and ecological processes (e.g., Kroeker et al., 2016) is essential to coastal decision-makers identifying ocean change management strategies (Chan et al., 2016). Furthermore, data managers should anticipate that their long-term time series will require intermittent redefinition. As the research focus of ocean change biology and ecology evolves beyond single-stressor and single-species experiments to multiple stressors at the ecosystem level, the processes for data archiving should scale as well, e.g., by incorporating new instruments with extended, standardized measurement descriptions. SBC LTER has maintained data products from moored instruments in a locally standardized format since its inception, and our handling and processing easily accommodates additional instruments. SBC LTER is currently using this same design process to incorporate data from new deployments for dissolved oxygen and phytoplankton fluorescence. Concomitantly with that process, we anticipate reorganizing our other moored products for more effective presentation and reuse, possibly adapting formats for easier integration of oceanographic data. Our existing framework for Durafet®-based pH time series data streamlines the incorporation of additional data streams by adding additional single deployment templates and building on the binned time series pattern. Our original design patterns were developed in consultation with researchers with similar projects (Gastil-Buhl et al., 2012), and adaptations to them will be carried out similarly. The development of easily handled datasets is immensely helpful to global ocean change researchers and would be nearly impossible without the input of data management professionals with a synoptic view of both the scientific research and the informatics landscape.

5. Conclusions

Autonomous pH sensor technology has equipped the marine science research community with the ability to quantify pH dynamics in numerous ecosystems, and future research efforts can utilize these data to inform studies related to the biological, ecological, and perhaps even economic impacts of OA. Ultimately, autonomous pH sensors can contribute remarkable power to scientists' abilities to investigate the consequences of OA. As the community expands its monitoring and observation efforts for a global view of changing ocean chemistry, it will be critical to coordinate and integrate data management practices. Our approach here serves as an example to other research groups

Table 3
Descriptions and status of pH data packages described in text and pertinent to development of pH data products of the Santa Barbara Coastal Long Term Ecological Research program. Refer to Table 1 for descriptions of design patterns and Fig. 1 for status.

| Name	Research goal	Primary data goal	Design pattern	Features	Status	Final published products
Coral reef study, pH from SeaFET	Short-term process study	Support a paper	None	Fringing coral reef, Moorea, French Polynesia	Publication 2011	knb.lter-mcr.2004
pH parameters from water samples	Field calibration of SeaFETs	Long-term time series, anticipated reuse	Benchmark samples	Sites supported by the several UCSB labs. Data added approx. annually	Initiated 2012, most recent publication 2014	knb-lter-sbc.75
pH parameters from SeaFET at four SBC LTER moorings	Characterize the near shore environment	Long-term time series, anticipated reuse	Binned time series	Four sites Data added approx. annually Enhancements planned in 2016 (see text)	Initiated 2012, most recent publication 2015	knb-lter-sbc.6001 knb-lter-sbc.6002 knb-lter-sbc.6003 knb-lter-sbc.6004
pH from ad hoc SeaFET deployments	Multiple short-term studies	Varies	Single deployment		Data set design	–
pH SeaFET deployments, for archive	Characterize the near shore environment	Archive	Single deployment	Packages added approx. annually Suitable for workflow input	Needs assessment	–
Stearns Wharf study, pH from water samples and SeaFET	Short-term process study	Support a paper	Benchmark samples	Frequent water sampling for TCO2, alkalinity	Needs assessment (awaiting completion of study)	–
Santa Cruz Island study, pH from SeaFET	Short-term process study	Support a paper	Single deployment		Publication 2016	knb-lter-sbc.93
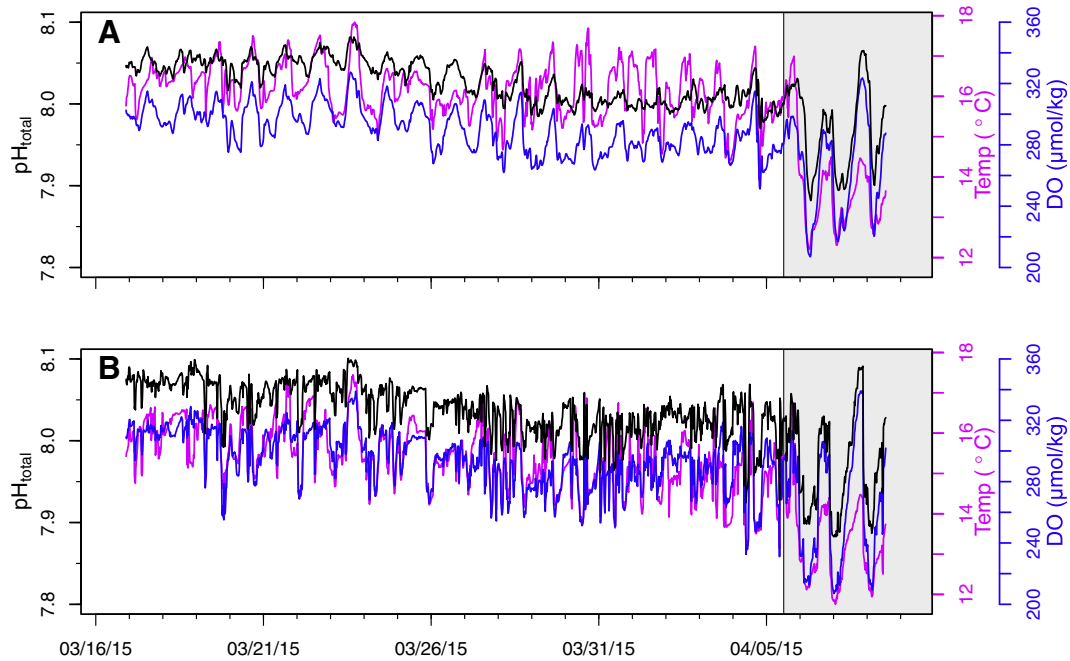
Fig. 5. pH, oxygen, and temperature time series collected by SeapHOxes (A) inside and (B) outside of a kelp forest show a complex multi-stressor scenario and stark differences in high-frequency pH variability over short spatial scales. Sites were 100 m apart, and sensors were moored 1 m from the bottom. Bottom depths were 7 m and 11 m, respectively. Gray shading indicates a period of upwelling.

dealing with the issue of managing OA-related oceanographic data to support ecological research. The data workflow we have developed easily accommodates the addition of new data to extend existing time series, can integrate pH data with other moored data, or be adapted for new instrumentation in the future. Collaborative data management expedites the process of generating publicly available data products while maintaining a format best suited to the data itself, and continued collaboration between researchers and data curators will remain an important linkage moving forward.

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