



# What sea-ice biogeochemical modellers need from observers

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## Abstract

Numerical models can be a powerful tool helping to understand the role biogeochemical processes play in local and global systems and how this role may be altered in a changing climate. With respect to sea-ice biogeochemical models, our knowledge is severely limited by our poor confidence in numerical model parameterisations representing those processes. Improving model parameterisations requires communication between observers and modellers to guide model development and improve the acquisition and presentation of observations. In addition to more observations, modellers need conceptual and quantitative descriptions of the processes controlling, for example: primary production and diversity of algal functional types in sea ice, ice algal growth, release from sea ice, heterotrophic remineralisation, transfer and emission of gases (e.g., DMS, CH<sub>4</sub>, BrO), incorporation of seawater components in growing sea ice (including Fe, organic and inorganic carbon, and major salts) and subsequent release; CO<sub>2</sub> dynamics (including CaCO<sub>3</sub> precipitation), flushing and supply of nutrients to sea-ice ecosystems; and radiative transfer through sea ice. These issues can be addressed by focused observations, as well as controlled laboratory and field experiments that target specific processes. The guidelines provided here should help modellers and observers improve the integration of measurements and modelling efforts and advance toward the common goal of understanding biogeochemical processes in sea ice and their current and future impacts on environmental systems.

## 1. Introduction

Understanding how sea-ice processes contribute to marine biogeochemistry is essential to accurately predict past, present, and future climate change responses of marine ecosystems in both the polar and global oceans. Sea-ice biogeochemical processes occur on very small spatial scales, confined to brine inclusions that are micrometers to centimeters in diameter within sea ice only a few meters thick. However, the horizontal scale is large, substance concentrations within the ice can be orders of magnitude larger than in the ocean, and at some times and locations sea-ice primary production can dominate the vertically integrated production. The dynamics of the sea-ice ecosystem directly affect those of the underlying waters down to the seafloor (Bluhm and Gradinger, 2008; Leu et al., 2015), but also affect the integrity of the ice, including porosity and radiative transfer (e.g., Krembs et al., 2011; Ewert and Deming, 2013). Through interactions and exchanges with both the overlying atmosphere and the underlying water, sea-ice biogeochemical processes may impact larger areas. Models of the entire Earth typically include sea ice but do not resolve the biogeochemical processes related

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to sea ice. Hence, the net effects on the climate system are far from clear. Contributions to the formation and emission of organic aerosols and greenhouse gases and effects on the carbon budget have also not been quantified yet. Ice algae likely have some measurable effect on regional scales but contribute little on a global scale (Kelley and Gosink, 1979; Legendre et al., 1992; Bluhm and Gradinger, 2008).

Developing numerical models of sea-ice biogeochemical processes is even more challenging than parallel efforts in the pelagic realm. The mixed solid-fluid sea-ice environment is distinctly different from the fluid pelagic regime, and both observational and modelling challenges are unique. Defining the fluid dynamics within the constrained sea-ice matrix is difficult, and there is a lack of non-destructive or remote sensing techniques for studying the sea-ice system (Garçon et al., 2014; Miller et al., 2015), i.e., satellite remote sensing techniques are not capable of measuring most properties within the sea-ice matrix.

Modelling sea-ice biogeochemistry is a relatively new field, but several reviews on physical and biogeochemical processes in sea ice are now available to initiate and guide model developments (Thomas and Dieckmann, 2010; Loose et al., 2011a; Vancoppenolle et al., 2013b; Vihma et al., 2013; Arrigo, 2014; Leu et al., 2015). These reviews confirm that the documentation of many sea-ice biogeochemical and small-scale physical processes is improving; however, their parameterisation in models is still relatively undeveloped. While there are many biogeochemical processes in sea ice worthy of investigation in support of a wide variety of goals, we, as sea-ice biogeochemical modellers, have identified a few processes of particular importance that require further field and laboratory studies: 1) incorporation and release of ice algal communities and nutrients (e.g., how is the ice algal community first established?); 2) controls and limits to primary production; and 3) the processes controlling the absorption and release of radiatively active substances, such as CO<sub>2</sub>, dimethylsulphide (DMS), and aerosols.

Many different types of observations are necessary to increase our understanding of sea-ice biogeochemical processes and allow us to incorporate them in models. Observations are also essential for the evaluation of biogeochemical models, including testing a model's sensitivity and skill (e.g., Deal et al., 2014). Global model systems create their own internal dynamics and cannot be expected to simulate a quantity exactly at all times and all places. Thus, the validation of these models is different than, for example, a limited area model that is constrained by forcing and boundary conditions (e.g., Oreskes et al., 1994), and their predictive capabilities are limited (e.g., Notz, 2014; Swart et al., 2015). Nonetheless, new and improved observations as well as ongoing research and analysis have led to improved climate models allowing for a better understanding of how climate processes work (Flato et al., 2013).

In spite of common goals and some mutual understanding of each other's needs, communication between observers and modellers needs to improve in order to reach those goals (Figure 1). It is clear that models or observations, taken alone, are not sufficient to improve global understanding of sea-ice biogeochemical processes and their impact on the large-scale climate system. Modellers need observations to evaluate and improve the models. The converse is also true: different types of models can help identify: 1) which processes are relevant for specific scientific questions; and 2) which are the likely spatial and temporal scales of variability of these processes. In this sense, models can be used as guides for future field campaigns, their locations, timing and the variables to measure. However, many barriers have hampered smooth communication between the two communities, including terminology and data formatting issues.



**Figure 1**

Conversation between a global climate modeller and an observer.

The choice of two polar animals together on one ice floe, when they do not co-occur in nature, is intended to represent the need for modellers and observers to meet at the same table, regardless of background.

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This paper is written from a modeller's perspective, albeit including insights from observers. We acknowledge that there are few people working at the extremes, who either only make observations or only do modelling, and that most researchers fall somewhere in between, using whatever tools they think are needed to address their research questions. However, it is also true that we tend to emphasize tools with which we are already comfortable, requiring higher levels of motivation to adopt new approaches. This paper is an effort to improve collaborations that will expand all of our tool kits, proposing ways to improve synergies between observing and modelling, while keeping in mind that the question is not, "How can the measurements improve our models?", but rather, "How can we use our models combined with your measurements to improve our understanding of the important biogeochemical processes occurring in sea ice?"

## 2. A need to maximize effective integration of observations and numerical models in sea-ice biogeochemistry

Sea ice acts as an interface, a reservoir, and a modifier in biogeochemical cycles, and observational data requirements may extend from the interior of the sea ice itself into both the atmosphere and the underlying water. Accordingly, observations of sea-ice biogeochemical processes must be a multidisciplinary effort. Also, model development should be a highly interactive process between modellers and observers. Evaluation, i.e., comparison of model output with observations to determine any bias between them, is an integral part of model development. However, long before evaluating a model, parameterisations based on process descriptions need to be developed. The conceptual description of processes is in many cases still a limiting factor in biogeochemical models, either because the process is not well known or because its complexity makes it computationally too expensive and challenging to validate. If the knowledge of the process is insufficient, the resulting parameterisation can be highly uncertain. Also, a specific process in a complex system rarely acts in isolation, though exactly that type of data is needed for validation. The kind of observations needed, and hence the effort required from the observer, varies with the model type and resolution, and with the question we seek to answer (Table 1). Whereas global and regional models require data sets covering all seasons and most of the model domain, preferably available as gridded datasets, one-dimensional vertical models focusing on representations of a seasonal cycle call for a long, data-rich (many types of measurements) time series at a specific location or from drift stations (e.g., as in the projects known by their acronyms SHEBA, ISPOL, CASES, SIMBA; Perovich et al., 1999; Lannuzel et al., 2008; Miller et al., 2011; Lewis et al., 2011). To develop specific parameterisations short, data-rich process studies with high temporal resolution, as well as controlled experiments, are also extremely useful (Section 3.1).

The current lack of field observations and the time lags between field programs limit our understanding of what processes need to be included in models. In that respect, sea-ice biogeochemistry lags behind oceanographic research, which is now benefiting from many decades of shipboard work and dramatic recent advances in tools for collecting data at high temporal and spatial resolutions (e.g., Gruber et al., 2010). Sea-ice biogeochemistry is not only a relatively new area of research, but the costs and challenges associated with sampling biogeochemistry within sea ice are substantial.

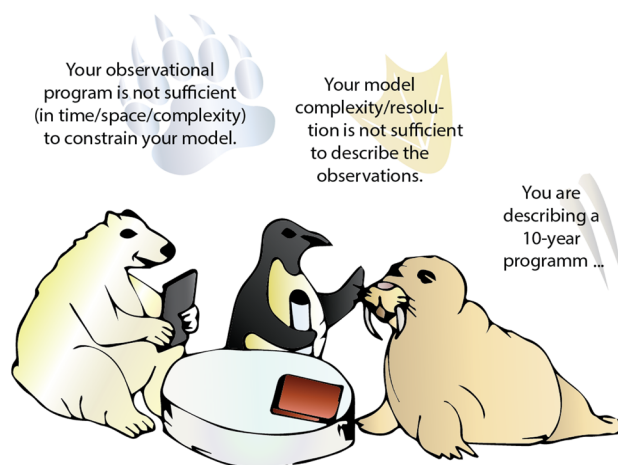
Generally, coordinated development of field programs hugely facilitates the collaboration between modellers and observers and involves writing proposals together, which in turn requires a common language and identification of common goals. Some large, interdisciplinary studies of the sea-ice environment have attempted to integrate observational and modelling needs from the beginning of the project design, but in the end, the results have not been integrated as well as hoped. More recently, however, several examples have generated constructive outcomes (e.g., projects known as BEST, SIMBA, INTERICE IV and Barrow 2009; Gibson and Spitz, 2011; Vancoppenolle et al., 2011; Moreau et al., 2014). An Arctic example of a project that has made progress towards coordinated collaboration between modellers and observers is the Forum for Arctic Modelling and Observational Synthesis (FAMOS, <http://web.whoi.edu/famos/>), which has evolved from the Arctic Ocean Model Intercomparison Project (AOMIP) and now includes marine biogeochemistry (Popova et al., 2012; Steiner et al., 2014, 2015).

Optimal collaboration between observers and modellers involves numerous feedbacks: 1) models inform the observational strategy; 2) observations are conducted and used to improve the models; and 3) new and improved models are rerun and used for data synthesis, interpretation, updated basin-scale and/or global estimates, and identifying/refining research questions (loop back to step 1). Many past projects have made the mistake of attempting to fully represent this multi-step process within a single research proposal, which typically

Table 1. Observational requirements for different model types

Model type	Example science questions	Information required from observers
Conceptual models	How do exchanges occur between sea ice and the surrounding systems? What nutrient sources or pathways are available to sea-ice communities?	Identification of required pools (e.g., required nutrient sources or detrital components, organism functional types (OFTs))
	How does the system work?	Qualitative interaction between groups and pools
Localized process models	How do exchanges occur between sea ice and the surrounding systems?	Observations from one location (field or laboratory)
	What controls sea-ice primary and secondary production?	High temporal resolution (hours–daily), particularly for transition times (freezing, melting)
	What controls fluid transport in sea ice?	High vertical resolution (1–10 cm for sea ice, 1–5 m for the upper ocean)
	How do processes occurring within surface brine skims and snow impact ice–air fluxes?	Details of community structure (OFTs)
	Can we quantify the rate of incorporation of particles associated with frazil ice into sea ice?	Measurements of rates, particularly for unresolved pools (e.g., bacterial consumption)
Regional models	Questions address balances of feedbacks and potential impacts of interactions between processes:	Spatially averaged quantities (range of 1–10 km <sup>2</sup> ) including information on spatial variability
	What is the contribution of sea-ice algae to the annual primary production in a particular area?	Some vertical averaging (10–100 cm for sea ice, 5–25 m for the upper ocean)
	How does ice–algal production affect the uptake or emission of climate active gases (e.g., Deal et al., 2011; Jin et al., 2012)?	Medium temporal resolution (days–months)
	How does brine rejection from sea ice contribute to carbon dioxide sequestration in the deep ocean?	Coarser grouping of pools
	How do sea-ice processes contribute and respond to ocean acidification?	Context: ancillary data (physical and environmental)
Global (climate) models	Questions address potential big-picture relevance of processes:	Spatially and temporally averaged quantities (10–100 km <sup>2</sup> ) including variance to determine uncertainty
	Will a decrease in sea-ice extent increase or decrease primary production in polar waters (e.g., Vancoppenolle et al., 2013a)?	Some vertical averaging (10–100 cm for sea ice, 5–25 m for the upper ocean)
	Does gas exchange in ice-covered regions affect the global carbon budget (e.g., Steiner et al., 2013)?	Lower temporal resolution (months–seasons)
	To what extent does brine rejection from sea ice contribute to carbon dioxide sequestration in the deep ocean?	Coarse grouping of pools (OFTs might have to include adaptive behaviour)
		Context: ancillary data (large scale physical and environmental conditions)

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**Figure 2**

Typical reviews of a grant proposal combining modelling and observations with reviewers from mixed backgrounds.

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must outline a plan that will take no longer than 3–4 years. However, because combining interdisciplinary modelling and observations is time consuming and, most importantly, iterative, the combined effort can easily extend beyond a typical funding framework (Figure 2). Therefore projects need to build on each other, both from the modellers' and the observers' perspectives.

This article focuses on the observational needs of sea-ice biogeochemical model development, but some basic guidelines apply to all modeller–observer collaborations throughout the earth sciences. For example, recommendations on the observational needs of climate models in polar regions, prepared by the Polar Climate Working Group (Kay et al., 2012) and a short note on observational needs for sea-ice models (Massonet and Jahn, 2012) also apply to sea-ice biogeochemical models. The fundamental starting point is that modellers and observers are both scientists. They share the same conceptual model and must understand each other's activities, and hence, they must develop a common language. Other points are:

- 1) quantities and units need to be consistently defined when comparing model fields and observations;
- 2) observed data need to be assessed for representativeness of the respective model output (data producers and users need to be “scale aware” in time and space);
- 3) gridded datasets need to meet commonly used standards for formatting meta-data to facilitate large scale model evaluation;
- 4) while regridding is often necessary to create difference maps, comparisons should be made on the original grid when possible; and
- 5) observations need to address key uncertainties affecting existing parameterisations or to help identify important processes that are not considered.

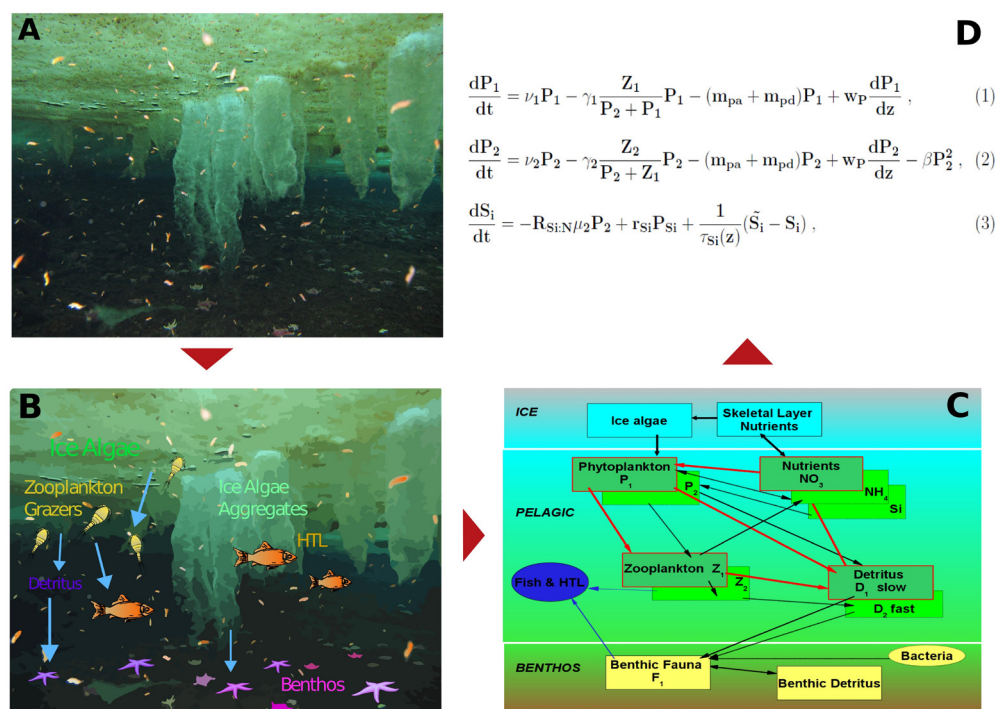
Kay et al. (2012) also articulated key uncertainties in integrating observations and model development. An expanded list of uncertainties that need to be identified and, if possible, quantified includes:

- uncertainties of analytical methods, including instrumental detection limits, accuracy, and variability;
- retrieval algorithm uncertainty;
- inconsistency in definitions;
- measurement reproducibility;
- inconsistencies between sampling and analytical methods;
- spatial variability (patchiness);
- temporal variability; and
- model internal variability.

Some of these uncertainties (a, b) can be reduced with technical and mathematical advances, which we will leave to the engineers, analytical chemists, and mathematicians. Other uncertainties (c, d, e) can be significantly reduced via concerted efforts on the part of observers (see for example Miller et al., 2015). Items f and g can theoretically be addressed by refining temporal and spatial resolution of the observations, but might be too difficult in practice. Some factors defy control and must simply be acknowledged (d, h).

Modellers particularly need to know uncertainties to constrain the ranges in parameter sensitivity studies (see below). It is important to know not only how large each of these uncertainties is, but also how the uncertainty was determined. For example, Stow et al. (2009) (their Figure 1) schematically indicate the skill of coupled marine biological–physical models by representing the relationships between model predictions,



**Figure 3**

From observations to numerical models.

The example given moves from a) Observed sea ice ecosystem (photo courtesy of Andrew Thurber, Oregon State University); to b) conceptual model of the sea ice-pelagic-benthic ecosystem; to c) schematic of a numerical sea ice-pelagic-benthic ecosystem model; and finally to d) numerical expressions (equations). HTL indicates higher trophic levels.

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observations, and the “true” state of the system with areas of uncertainty around them. The higher the overlap of those areas, the higher the skill. Some uncertainty ranges can be provided reasonably accurately (e.g., instrumental precision), whereas others can be calculated from regional or temporal averages (some modellers prefer to receive observational data as raw as possible to avoid inconsistencies in error definitions).

### 3. How modellers use observations to develop models

Before going into more detailed recommendations, we describe how sea-ice biogeochemical modellers use observations in developing models. Models in general are representations of selected components of the natural system and can take multiple forms; e.g., theoretical constructions, schematic descriptions or numerical equations. A biogeochemical model can be made up of several components, which we refer to as modules. Here we use the development of a numerical ice algae-pelagic ecosystem module as an example; a parallel process would be applied for developing other biogeochemical modules, carbon or sulphur cycling, pollutant transport, etc. The fundamental purpose of a numerical model is to represent the essential behavior of a natural system with simplified numerical formulations (equations). Figure 3A shows a photographic image of a natural sympagic-pelagic-benthic ecosystem, which we use as a starting point. Based on the observations of this natural system, scientists (both modellers and observers) construct a theoretical framework based on concepts; e.g., which are the main pools, how do they interact, and what is their relationship to the physical environment (e.g., ice algae form a distinct pool, ice algae grow at the bottom of the ice, ice algae are eaten by zooplankton, some ice algae die and sink to the bottom, etc., Figure 3B). From this conceptual model, a model schematic can be created, which represents the identified pools and their interactions in form of boxes and arrows (Figure 3C). From this model schematic, parameterisations are proposed or can be derived and expressed in the form of numerical equations (selected examples are given in Figure 3D). Variables represent the pools (boxes), and functional dependencies on time represent the interactions between the pools (arrows). The number of boxes and arrows determines the complexity of the model (e.g., Gentleman, 2002; Denman, 2003; Le Quéré et al., 2005). The functional dependencies contain parameters which can in turn depend on single or multiple variables (bio-geochemical or physical). Once the numerical model is formulated and executed, the model output is compared with observations (preferably different observations from those used to develop the parameterisations) to evaluate the model’s performance. Based on the outcome some model parameters might need to be better constrained (the model needs to be “tuned”). To finalize a version of a model or a single module, multiple revisions to each stage might be necessary and new observations can instigate revisions at all stages leading to a revised model version. The uncertainties associated with parameter values can be the largest contributor to the total uncertainty of the model output, particularly if the external forcing is well constrained. Hence specific observations to refine individual equations might be required.

Moving from conceptual models to numerical parameterisations requires generalized quantification of processes, something which is lacking for many sea-ice biogeochemical processes. One example is the finding that melting sea ice enriched in iron and organic matter contributes to pelagic ice-edge phytoplankton blooms in the surface ocean (Lancelot et al., 2009; Lannuzel et al., 2013; Wang et al., 2014). While mesocosm experiments confirm the process, field observations remain unclear on the specific mechanism and thus on the large-scale importance of such ice-associated iron fertilization. This lack of either a mechanism or a generalized rate term directly linking ice melt to pelagic primary production constitutes a significant hurdle in model development and limits our ability to resolve the complexity of Southern Ocean ecosystems.

Sea-ice ecosystem modellers have benefited from the availability of pelagic ecosystem models, which can be adapted to create a first-order sea-ice ecosystem model by assuming that the biogeochemical processes are the same in both systems. This approach has been suggested by Tedesco and Vichi (2014) to encourage ecosystem modellers of polar regions to add a new sea-ice ecosystem component to their modelling frameworks. However, while this assumption of comparability may be true for the structural relationships between some processes (e.g., nutrient uptake, photosynthesis, respiration, remineralization, excretion), the rates of these processes can be different, either universally (sea ice versus pelagic) or regionally. Some processes may also be fundamentally different or exclusive to one environment; e.g., physical transport processes are very different in these two mediums.

Finally, model evaluation and skill assessment (Stow et al., 2009) are required both to develop models and to know the level of confidence we can have in the results. Biogeochemical models produce three kinds of data that can be evaluated via comparison with observations (Franks, 2002): 1) prognostic model variables (Figure 3C, model boxes; i.e., concentrations); 2) rates/fluxes (Figure 3C, model arrows; e.g., growth, mortality); and 3) derived or secondary quantities (diagnostic variables, e.g., chlorophyll-a (Chl<sub>a</sub>) in nitrogen-based ecosystem models). Evaluation and skill assessment can be performed using any of those quantities for which observations are available.

### 3.1. Model types

Different types of models have different data requirements for both model development and evaluation. The specific questions addressed determine both type and complexity of the model, which in turn determine the required observations. We propose that, in a general sense, every process can be written as an equation and hence models can address any question, given that the required observations can be made. Putting the steps into a sequence, the first is to articulate the question one wants to answer, and the second is to design the model and the required sampling program. The most significant limitations, therefore, are generally on the observational side; e.g., can the parameters, fluxes, etc. be measured? The observational needs for the validation and, to a certain extent, development for each type of model, as well as some example science questions are given in Table 1.

Conceptual models are theoretical constructions made of concepts, used to help understand a system (natural or not), to which every scientist (modeller and observer) contributes (Figure 3B). Numerical implementations of such a common, conceptual model then form a numerical model. Conceptual models need information on pools, fluxes, community structure, and behavior. In addition conceptual models require coincident descriptions of the physical environment, along with the biogeochemistry and some ideas about how they are connected. A process might be deemed unimportant or insufficiently known to be included. When a conceptual model is used to guide the development of a numerical model, we also need to take into account that a greater number of parameters causes more uncertainties and requires more computation time. These disadvantages need to be weighed against the gain from including a process (e.g., including a process can also help reduce the uncertainty in a parameter by providing a physical or biogeochemical basis for variability that is measurable or specified by known quantities). If too many parameters are uncertain, the model loses predictive capabilities, although it can still be a useful tool for investigating uncertain processes.

0-D/1-D models focused on process studies are designed to develop parameterisations, and require a quantitative understanding of the processes in question, in addition to a conceptual framework. These models require site-specific variables, rates and the variations in both over time from field or laboratory experiments, preferably with multiple replicates to constrain uncertainty ranges. These models cannot reproduce processes that are not understood quantitatively at least to some extent. Linking 0-D/1-D model development with laboratory experiments can be particularly productive. Taking the example question “Can we quantify the rate of incorporation of particles (biogenic or lithogenic) associated with frazil ice into sea ice?”, the model development can run in parallel with the experiments. The laboratory settings and observations (e.g., air temperature, mixing, growth rate, crystal size, presence of living organisms, etc.) can be tuned in the model to evaluate which individual parameters exert the most control over the scavenging process, and then the laboratory settings can be varied to test the predictions from the model.

Often information about an individual process is distributed among several individual studies and papers. If there are many such studies, synthesis or review papers summarizing the observed results and conceptual models are extremely valuable to the modelling community.

To develop equations, observed turnover times or rates are generally more useful than measured variable concentrations. In cases where fluxes are not directly measured but estimated from changing concentrations, the expertise observers bring to the estimation of these fluxes is invaluable in developing meaningful representations in models.

Regional models or regionally focused global models need spatially averaged variables and rates, including information on spatial and temporal (seasonal, inter-annual) variability. Often a specific time of the year is particularly important for a process, but is severely underrepresented in the observations (e.g., the autumn period of sea-ice formation or the final stages of sea-ice melt during the spring-summer transition). Because observational data are often unevenly distributed in space and time, data products (i.e., climatologies) used to evaluate model output can be biased. For example, repeat surveys generally follow some spatial pathway several weeks in different years, and the temporal vs. spatial control over the observed variations is rarely clear. Hence, a description of the potential biases is important for modellers using these products.

Matching model output at a specific location with an individual observation at the same location and time of year is particularly difficult if the variability in the observations is high and the number of data points per grid cell is small. Essentially, regional model output provides values representative of each simulated grid cell, averaging over the spatial variability within the grid cell. If the variability within the grid cell is greater than the differences in averages between grid cells, a single data point will not be useful in evaluating the model. On the other hand, time series measurements from single sites can provide valuable information to help evaluate regional models, giving insight into the annual cycle, vertical profiles, and interannual variability (e.g., Doney et al., 2009).

Global climate models and Earth system models (ESMs) contain fully coupled atmosphere, ocean, sea ice, and land components, with ESMs also including interactive biogeochemical modules for all components. While much of the parameterisation development happens within the models described above, evaluating global model performance (e.g., Flato et al., 2013) requires spatially and temporally averaged variables and rates, including information on uncertainty. Multi-model simulations are also commonly used for evaluating climate model projections (see 3), in Section 3.2, below). The model spread in multi-model simulations is indicative of uncertainties associated with natural internal variability of the climate system and structural and parametric uncertainty in the climate models considered (Sillmann et al., 2013). Comparing the multi-model spread with the uncertainty ranges in the observations allows us to further assess the robustness of the model projections.

### 3.2. Model development tools and observations

Often, sufficient observations for thorough model evaluation are lacking, or the nature of the model does not allow point-to-point evaluation. In these cases, at least three classes of tools are available for further model development.

Model sensitivity studies assess the impact of specific processes or parameters on the whole system and evaluate the variables to which the system is most sensitive. Testing the sensitivity of a parameter over a certain range allows for an estimate of the importance of a certain process compared to another and can identify parameters that need to receive focused observational attention to reduce the overall uncertainty of the system. The parameter range for a sensitivity study is set by the range of the measurements or an estimate of the uncertainty in the parameter, which are thus important to report.

Ecosystem modellers also use tools such as standard optimization algorithms (e.g., Ward et al., 2010), weak constraint and assimilation parameter estimation (e.g., Losa et al., 2004; Simon and Bertino, 2012), and Bayesian models (e.g., Malve et al., 2007; Jones et al., 2010; Weir et al., 2013) to tune parameters in systems that are only weakly constrained by observed data. These parameter estimations generally improve with better a priori information; i.e., our estimates and assumptions of how ecosystem variables may be linked. Accordingly, these optimization tools improve as our conceptual models improve.

Model intercomparisons are useful to identify robust processes and features and determine model uncertainty. Detailed model intercomparison exercises involving polar biogeochemical models are limited due to many developmental gaps, measurement-based uncertainties, and low model resolutions, which prevent simulation or reproduction of specific patterns at specific points in space and time. Alternatively, model intercomparisons can focus on features that are characteristic of the investigation area, such as the deep chlorophyll maximum in the Arctic Ocean (Steiner et al., 2015). These intercomparisons require an observational data set for evaluation (Table 1), as well as an appropriate forcing data set (atmospheric and oceanic environmental variables for at least the time period of the observations in sufficient resolution for the process time scale in question; e.g., diel, seasonal).

## 4. Relevant variables: Status and open questions

Sea-ice biogeochemistry is highly important on the local scale and plays a key role in polar elemental cycling with potentially large-scale impacts that need to be understood (Shepson et al., 2012). The development



Table 2. Values for common biological parameters of state-of-the-art sea-ice models

Model reference	Mean Chl <i>a</i> specific attenuation coefficient	Photosynthetic efficiency	Half-saturation constant for Si uptake	Maximum ice algae growth rate	Chl <i>a</i> :C ratio
	$a^*$	$\alpha^0$	$b^s$	$r_0$	$\theta_{chl}^0$
	$\text{m}^2(\text{mg Chl}a)^{-1}$	$\text{mg C}(\text{mg Chl}a)^{-1}$ ( $\mu\text{E m}^{-2}$ ) <sup>-1</sup>	$\text{mmol Si m}^{-3}$	$\text{day}^{-1}$	-
Arrigo et al. (1993, 1997)	-	-	-	1.44	-
Lavoie et al. (2005); Pogson et al. (2011)	0.02	$8.3\text{e}^{-6} - 33.3\text{e}^{-6}$	4.0	computed	-
Nishi and Tabeta (2008)	-	-	7.0	2.0	0.05
Jin et al. (2006, 2007, 2012); Deal et al. (2011); Ji et al. (2013)	-	-	4.0	1.44	0.033
Tedesco et al. (2010, 2012); Tedesco and Vichi (2014)	0.001	$1.8\text{e}^{-6} - 3.8\text{e}^{-6}$	0.1 <sup>a</sup>	1.5 – 2.0	dynamic
Sibert et al. (2010, 2011)	-	$16.6\text{e}^{-6}$	-	0.08	0.1
Dupont (2012)	-	-	-	1.5	-
Elliott et al. (2012)	0.03	-	4.0	1.5	-
Saenz and Arrigo (2012, 2014)	-	-	60	0.81	0.0286
Moreau et al. (2015); Vancoppenolle and Tedesco (2015)	-	-	-	0.86 – 1.56	0.01 – 0.05

<sup>a</sup>in units  $\text{mmol Si m}^{-2}$ 

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of sea-ice biogeochemical models is relatively recent, and many processes are ‘undermodelled’ (i.e., only limited or no modelling efforts to describe the process have been undertaken). While our observational data base of sea-ice biogeochemical variables is slowly increasing, many processes are insufficiently known to warrant implementation in models, and for the processes that are included in models, the magnitudes of the applied parameters are not well constrained. A selection of commonly used biological parameters in state-of-the-art sea-ice biogeochemical models indicates the large uncertainties and lack of standardization for these parameter values (Table 2). While the available models of sea-ice biogeochemistry frequently use the same or similar values for their parameters (e.g., C:N or Chl*a*:N ratios; nutrient half saturation constants; temperature coefficients for growth, respiration and remineralisation), this communality is not necessarily indicative of general agreement and sufficient knowledge. A more detailed list of parameters used to date is beyond the scope of this paper. Instead, we choose to highlight areas that we think are most critically in need of additional observations.

#### 4.1. Ice algal incorporation and release

There is an urgent need for research on the mechanisms by which microbes (algae, bacteria, and protozoa) are incorporated into forming sea ice, as well as potential vertical displacement during ice growth (“upward growth”). Typically, we lack observations from autumn (Leu et al., 2015), due to numerous logistical challenges, and algal incorporation into new sea ice has been included in sea-ice biogeochemical models only very simplistically (e.g., specification of initial Chl*a* concentration at ice formation; Lavoie et al., 2009). Even though theories on algal entrapment are over 30 years old (e.g., Garrison et al., 1983, 1990, 2003), the processes are still not well understood or quantified. Most of the published work is based on sea-ice formation experiments (e.g., Giannelli et al., 2001; Aslam et al., 2012; Eronen-Rasmus et al., 2014; Zhou et al., 2014; Jørgensen et al., 2015), although some field-based data are now emerging (Janssens et al., 2015). Recent studies have demonstrated selective incorporation of large cells in forming sea ice, which could be favored by production of extracellular polysaccharide substances (EPS or exopolymers); (Gradinger and Ikävalko, 1998; Riedel et al., 2007; Różanska et al., 2008; Becquevort et al., 2009; Janssens et al., 2015) and bacteria may be incorporated into forming sea ice via attachment to algae or larger detrital material (Grossmann and Dieckmann, 1994; Weissenberger and Grossmann, 1998; Riedel et al., 2007; Meiners et al., 2008). However, the degree of stickiness of sea-ice algae remains largely unexplored and this information is of limited help in developing parameterizations for particle entrapment in ice during the fall. Quantitative measurements are needed to parameterize the relationships between ice growth rate, ice texture, cell sizes and numbers of cells, and exopolymer concentrations. Efforts to ultimately understand the processes by which cells are incorporated

into newly-forming ice would be most efficient if autumn-based field studies, laboratory experiments, and modelling were combined.

The release of ice algae from sea ice is an important link between the sea-ice, pelagic and benthic ecosystems. Ice algal export under frequently changing conditions depends on numerous factors in complex ways (Michel et al., 1996, 2002; Krembs et al., 2001; Lavoie et al., 2005; Vancoppenolle et al., 2007, 2010; Tison et al., 2008, 2010; Krembs et al., 2011; Arrigo, 2014) and may contribute to the spatio-temporal patchiness of biogeochemical variables in sea ice (Juhl and Krembs, 2010). However, most models currently formulate ice algal release simply as proportional to bottom ice melt rate, which is determined by thermodynamics. All of the processes contributing to ice algal release to the water column warrant further testing in order to develop and critically evaluate model parameterisations. Many of the questions relating to entrapment, incorporation, and release of cells also apply to other biogeochemical parameters.

## 4.2. Controls on primary production in sea ice

Primary production in sea ice generally depends on a multitude of factors; e.g., which species accumulates or colonizes the ice during its formation (see above), and how they survive in winter and grow in other seasons (depending on ambient ecological conditions such as temperature, salinity, space, light, and nutrient availability). One of the most immediate questions is, what limits primary production? At the base of the ice, algal growth appears to be controlled by the interplay between light and nutrient supply. The controlling factors are less clear in brine inclusions higher up in the ice.

### 4.2.1. Light

Although ice algae are adapted to low light levels (e.g., Arrigo et al., 2010), the specific levels at which primary production ceases or at which different types of ice algae start to grow within the ice are poorly constrained (Gosselin et al., 1985; Cota and Sullivan, 1990; Kirst and Wiencke, 1995; Gradinger, 2009; Leu et al., 2015). Nonetheless, the available light has a major effect on the onset of and maximum in ice algal growth (Watanabe et al., 2015). In addition, the characteristics of both the ice and the overlying snow dramatically influence the amount and nature of the light available to sea-ice algae (e.g., Mundy et al., 2007; Light et al., 2008; Frey et al., 2011; Castro-Morales et al., 2014; Katlein et al., 2014; Leu et al., 2015).

While one reason for biases in modelled sea-ice primary production is likely that the models do not simulate the amount of light appropriately, it is also possible that modellers do not assign the proper light parameter (usually the value of the initial slope of the photosynthesis-irradiance curve) to the group(s) of algae they are modelling. In observational studies in the Arctic (Leu et al., 2015), light appears to be the main limiting factor at the beginning of the growth season, and nutrients become limiting at a later stage, a pattern which has been represented in the models developed for sea ice in the Arctic (Lavoie et al., 2005). However, improvements in the representation of light transmission lead to distinct improvements in the modelled light availability affecting onset and continuation of ice algal growth (e.g., Lecomte et al., 2011; Pogson et al., 2011; Vihma et al., 2013; Abraham et al., 2015).

The interplay between light and nutrient control on the sea-ice communities depends not only on seasonal, but also on spatial parameters (i.e., at a given time, surface, interior, and bottom communities are limited by different factors). Sea-ice biogeochemical models that only include undifferentiated algal biomass confined to the bottom of the ice cannot accommodate such relationships. For example, improved light conditions during snow melt can also affect ice communities within the upper ice matrix or in gap layers (Arrigo, 2014). Therefore, model parameterizations might be required to allow growth further up in the ice (Tedesco et al., 2010; Pogson et al., 2011; Duarte et al., 2015).

Improved high quality observations of radiation in relation to snow and ice properties and distributions are essential to ultimately parameterize light availability in sea-ice models. New types of instrumented platforms, such as ice-tethered profilers (Laney and Sosik, 2014) and autonomous submarines (Nicolaus et al., 2013), now provide valuable information of the light available under sea ice. Despite the absence of direct measurements in the ice column, these measurements allow for some estimates of the light field within the ice, if light absorption in the ice algal layer can be accounted for.

### 4.2.2. Nutrients

Complete exhaustion of all four macro-nutrients (nitrate, silicate, phosphate, and ammonium) has been documented in sea ice, but is usually limited to sections cut off from potential resupply from the underlying water (Thomas and Dieckmann, 2002). For ice algae, some studies report nitrogen (e.g., Cota et al., 1987; Gosselin et al., 1997) or phosphate (Becquevort et al., 2009) limitation, but most studies highlight silicate limitation (e.g., Gosselin et al., 1990; Smith et al., 1990), because of its lower remineralisation efficiency (Lizotte, 2003). Hence, some models chose to use silicate as the prime nutrient for ice algal regulation (Lavoie et al., 2005; Tedesco and Vichi, 2014). This generalization assumes that diatoms are the key functional group for ice algae. If different phytoplankton species without silica walls (e.g., dinoflagellates, as recently observed

to dominate interior austral summer sea-ice, Torstensson et al., 2015) are included, this simplification is no longer applicable. The choice of the limiting nutrient might also be location-dependent; e.g., nitrogen might be more appropriate in low nutrient regimes like the Beaufort Sea (Lavoie et al., 2010). Nutrients are provided to sea-ice communities through exchange with the seawater by convection at the ice/water interface, infiltration into the snow pack, and/or by brine transport within the ice. Models tend to use different approaches to represent nutrient supply, depending on their complexity (e.g., Vancoppenolle et al., 2010).

Measurements are also still lacking as to how much primary production can be sustained by remineralized nutrients within closed brine pockets (Fripiat et al., 2014) and to what degree ice algae and bacteria compete or cooperate. Even though information on heterotrophic activity in sea ice is available (Deming, 2010; Bowman, 2015), at this point bacterial remineralization rates are treated as constants or vary only with temperature in most, if not all, models. Input is needed from observers to evaluate the validity of these approaches. To our knowledge, viruses have not yet been implemented in any sea-ice model, and more quantitative information about their role in sea ice is still needed (Deming, 2010).

The micronutrient iron and its dynamics in sea ice have widespread implications for pelagic productivity, particularly in the Southern Ocean, and presents a special case for sea-ice biogeochemical modellers (van der Merwe et al., 2009, 2011; Aguilar-Islas et al., 2008; Lannuzel et al., 2007, 2010, 2014; de Jong et al., 2013; Kanna et al., 2014; Wang et al., 2014; Janssens et al., 2015). The mechanisms of Fe incorporation into sea ice still need to be quantified, as well as the potential coupling between Fe and organic matter, the magnitude of the estimated fluxes in relation to the timescale of the measurements, the residence time of the Fe once released into seawater, and whether the particulate Fe in sea ice is bio-available.

The modelling studies by Lancelot et al. (2009) and Wang et al. (2014) represent Fe dynamics in sea ice without including biological or chemical processes within the ice. The Fe uptake values had to be tuned, based on the limited observations of distributions available. Both studies highlight the necessity to include Fe transport by sea ice to adequately simulate open ocean primary production in the Southern Ocean and illustrate well how models can be used to test hypotheses from field studies and further promote observations.

Nutrient transport and supply processes in sea ice are ideal subjects for combined field, laboratory, and model studies, and much progress has been made in support of modelling nutrient transport within sea ice (Untersteiner, 1968; Golden et al., 1998; Becquevort et al., 2009; Notz and Worster, 2009; Vancoppenolle et al., 2010; Wang et al., 2014).

#### 4.2.3. Other factors

Representative measurements of Chl $\alpha$ :C ratios for sea-ice communities are required to properly estimate total carbon biomass (e.g., Tedesco et al., 2012). We acknowledge that Chl $\alpha$  is not always a good proxy for algal biomass, especially when light is limiting, and more information on how the Chl $\alpha$ :C ratio varies with light conditions would be beneficial. Measurements of elemental (i.e., C:N:P) ratios in sea ice, another key ratio needed to understand the relationships between production parameters, are needed, particularly to decide whether the ratios should be held constant or varied with environmental conditions in a model. Information on the timing and conditions of grazing on ice algal biomass is also insufficient (Krembs et al., 2000; Lavoie et al., 2005; Watanabe et al., 2015). In addition, we need a better conceptual understanding of the ways in which shorter ice seasons may restrict the sea-ice algal bloom period (Lavoie et al., 2010; Tedesco and Vichi, 2014). It is also not clear how pH (including anthropogenic ocean acidification processes; AMAP, 2013) may affect ice algal primary production.

#### 4.2.4. Functional Types (FT) versus species

The simplest sea-ice ecosystem models consider only one group of algae (i.e., diatoms) and often only one limiting nutrient. However, observations show that a variety of photosynthesizers and sea-ice heterotrophs are normally present in sea ice (e.g., Deming, 2010; Pedrós-Alió et al., 2015; Bowman, 2015). Although computational costs may encourage simplistic representations, an expansion in ecosystem complexity might be needed to represent the various communities growing at different locations within sea ice and through the seasonal progression (Tedesco and Vichi, 2014), and to assess how those communities contribute to fluxes of climatically active gases and aerosols. Models of the formation of platelet ice are slowly emerging (Wongpan et al., 2015), but more complete descriptions of both platelet (Arrigo et al., 2010) and under-ice strand communities (Arrigo, 2014) are also needed to advance models of total sea-ice primary production. While modellers have a tendency to oversimplify the system, observers often provide details at a level that cannot be addressed by models. Presenting the community composition in terms of functional groups would aid the development of meaningful models. Functional groups identify organisms serving the same ecological and physiological roles in a certain environment. These roles are represented in models using the same parameters. A common, useful trait of functional groups in models is cell size, which can be efficiently analyzed by flow cytometers, whereas more time-consuming microscopy often provides a level of detail that is not useful in model development. Traits include calcification and DMS production.

### 4.3. Fluxes of climatically active gases and aerosols

The porous nature of sea ice provides a habitat for ice algae as well as a pathway for exchange of organic matter, nutrients, and gases with the seawater below and the atmosphere above through air-ice and ocean-ice gas exchange, brine drainage, and seawater entrainment (Loose et al., 2011a). The physical, biological, and chemical pathways (and their rates) by which sea ice affects the distribution of biogenic gases (such as CO<sub>2</sub>, O<sub>2</sub>, CH<sub>4</sub>, halogens and DMS) between the ocean and the atmosphere are of interest to modellers studying the global carbon cycle and climate change.

#### 4.3.1. Gas flux parameterisations

A number of field programs have measured gas fluxes above sea ice in both the Arctic and Southern Oceans (Semiletov et al., 2004; Zemmelen et al., 2006, 2008; Nomura et al., 2010a, 2010b, 2012, 2013; Else et al., 2011; Miller et al., 2011; Papakyriakou and Miller, 2011; Sejr et al., 2011; Geilfus et al., 2012, 2013, 2014, 2015; Muller et al., 2012; Barber et al., 2014; Delille et al., 2014; Sørensen et al., 2014; Brown et al., 2015; Fransson et al., 2015), but formulating gas exchange in ice-ocean biogeochemical models is not straightforward. In the absence of specific gas-exchange parameterisations for the sea-ice environment, some sea-ice researchers have used parameterizations developed for open water conditions (e.g., Trevena and Jones, 2012). However, as noted by Rutgers van der Loeff et al. (2014), applying open water approaches to ice-atmosphere fluxes causes scaling problems. For example, many ocean-atmosphere gas exchange coefficients have been determined under conditions of large fetches and therefore are not applicable to brine-air exchange. A number of studies have begun to develop parameterizations for ice-air gas exchange (Loose et al., 2011b; Crabeck et al., 2014; Sørensen et al., 2014), but the universality of those formulations is still unclear. In a recent study Moreau et al. (2014) modelled the ice-atmosphere gas fluxes as a diffusive process, which requires more information about the molecular diffusion coefficients for gases within the sea-ice column. Large variations in measured ice-atmosphere gas fluxes and differences between the values from eddy covariance and chamber measurements (Miller et al., 2015) make it difficult for modellers to constrain their parameterisations or even the environmental factors contributing to the flux. For example, the placement of a flux chamber blocks wind pumping, which is likely an important factor driving fluxes in undisturbed environments (Bowling and Massman, 2011), whereas eddy covariance measurements have a much larger footprint (several hundred m<sup>2</sup>) and include the effects of larger scale ice variability, including potential cracks (Moreau et al., 2015), as well as boundary layer processes, such as those occurring within the snow cover. Direct air-ice gas exchanges are generally lower than air-sea exchanges, but Loose et al. (2009) and Else et al. (2011) found that in a mixed ice-water environment, fluxes are much higher than over open water. Models generally do not represent this flux enhancement in broken, mobile sea ice and generally scale down fluxes estimated from open-water parameters by the ice area fraction (Steiner et al., 2013). Until a comprehensive conceptual understanding of the origins of sea ice-air gas fluxes and generalized flux parameters (e.g., gas transfer velocity, diffusivity) covering the variety of sea-ice environments and conditions are available, estimates of the spatial and temporal variability in gas fluxes from sea ice and seawater in ice-covered environments (e.g., Nomura et al., 2013) are useful for determining whether model results are within expected ranges.

#### 4.3.2 DMS and other organic aerosols with sources in sea ice

The climatically active gas dimethylsulfide (DMS), contributes to organic aerosol production and cloud formation in the marine boundary layer (Quinn and Bates, 2011; Levasseur, 2013). The DMS precursor, dimethylsulfoniopropionate (DMSP), acts as an osmolyte and can be produced in large amounts by sea-ice algae exposed to high salinities (Trevena and Jones, 2006). In areas where terrestrial open-water sources of atmospheric aerosols are limited, sea-ice DMS emissions might be an important contributor to the total aerosol production (Levasseur, 2013). However, large areas of both polar oceans remain unexplored in terms of DMS cycling and fluxes. Although additional measurements of DMS concentrations in sea ice will be valuable, more importantly, modellers need the rates at which DMS is produced and degraded by the sea-ice community as well as DMS fluxes to the atmosphere to fully develop and adequately evaluate DMS biogeochemical models for ice-covered seas. Sensitivity studies of DMS models (e.g., Jodwalis et al., 2000; Steiner and Denman, 2008; Elliott et al., 2012) applied to sea ice may suggest which processes are key to governing DMS emissions in and around sea ice and can contribute to designing field and laboratory investigations.

#### 4.3.3. Other gas-related processes

Gas bubbles in sea ice (e.g., Matsuo and Miyake, 1966; Light et al., 2003) likely form as ice brines become supersaturated (Carte, 1961; Lubetkin, 2003). Little is known about their nucleation rates, but Moreau et al. (2014) used a modelling sensitivity analysis to show that nucleation rate is important to accurately represent argon dynamics. Argon transport due to buoyant rise of gas bubbles (Zhou et al., 2013) has also recently been modelled (Moreau et al., 2014, 2015), but additional observations, particularly of the impact on other gases, are needed to constrain the model parameterisations.



In addition, the biological consumption and release of climatically active gases from sea ice is still largely unknown. At this point, the role of primary production and respiration in  $O_2$  and  $CO_2$  dynamics is modelled using standard stoichiometric Redfield ratios, assuming that biological activities are reasonably well represented in models. The role of ikaite ( $CaCO_3$ ) in  $CO_2$  dynamics in sea ice (e.g., Geilfus et al., 2013), including the rates of precipitation and dissolution (Hu et al., 2014; Papadimitriou et al., 2014) are only beginning to be constrained. Finally, the thermodynamic parameterizations used to calculate carbonate chemistry in seawater solutions are generally not valid under sea-ice brine conditions (Brown et al., 2014), but until the corrections required to apply the constants in sea ice are determined, we are limited to extrapolating the existing seawater expressions beyond their empirical limits (e.g., Delille et al., 2007).

In the Arctic, where methane is released as gas bubbles from anoxic shelf sediments (e.g., Shakhova et al., 2009), sea ice is also an important player in ocean-atmosphere methane fluxes. Methane production also seems to be associated with low N:P ratios in the surface waters when sea ice is present (Damm et al., 2010; Kort et al., 2012). The mechanisms controlling methane releases to the atmosphere and the rates at which they occur need to be identified before their large scale impacts can be estimated with models. Finally, although surface brine skims and frost flowers have been implicated in fluxes of numerous sea-ice chemical species (e.g., Ewert et al., 2013; Geilfus et al., 2013; Granfors et al., 2013; Bowman et al., 2014), the conditions controlling those fluxes, as well as their rates, are still unclear. In particular, the surface of the sea ice can be a strong source of tropospheric bromine monoxide (BrO) and other halogens (Rankin et al., 2002). Saline snow and ice surfaces (e.g., frost flowers) provide the halides for heterogeneous production of reactive halogen gases, such as BrO (Simpson et al., 2015), but the implications for the predictability of bromine explosions are still very uncertain.

## 5. The necessity of context

### 5.1. Ancillary measurements and data reporting

A recurring point for modellers, as well as for everyone else, when using and interpreting observed data, is the requirement for ancillary measurements to go with biogeochemical data. Modellers' efforts benefit hugely from simultaneous sampling of biogeochemical observations and measurements of the physical properties of the sea ice and its bounding media (Eicken et al., 2009; Miller et al., 2015). The rate of change of any variable results from both physical and biological processes. Hence, while any observation is valuable, as much physical context as possible should be provided (e.g., information on temperature, salinity, ice texture, ice/snow thickness, irradiance, wind speed and direction, atmospheric boundary layer height, and ocean mixed layer depth can provide useful context for the biogeochemical measurements). For example, to parameterize nutrient supply mechanisms (i.e., fluxes between water and sea ice) we need to know: mixing coefficients and nutrient concentrations in the mixed layer, as well as under-ice roughness; brine volumes and structures that affect fluid transport within sea ice and regulate exchanges with under-ice waters; information on snow cover and freeboard as required to assess seawater infiltration at the snow/ice interface, and therefore nutrient supply to surface communities; and nutrient consumption as controlled by the timing and magnitude of algal growth, which in turn depend upon the photosynthetically active radiation (PAR) received and nutrient availability (Lavoie et al., 2005; Tedesco et al., 2010; Pogson et al., 2011). Brine salinity and temperature also affect the physiological responses of sympagic organisms (Tedesco and Vichi, 2014). Since biogeochemical processes, particularly ice algal primary production and inorganic carbon dynamics, can be quite variable over the vertical extent of a sea-ice floe, it is important to divide an ice core into sections and report the appropriate section averages for the entire core in relation to the total ice thickness (e.g., bottom 5 cm of a 76 cm ice core). To address spatial heterogeneity, multiple ice cores (at least duplicate) should be analyzed from a single ice floe or within a specific area (Miller et al., 2015). Finally, fundamental differences in ice structure related to the circumstances under which sea ice forms and its subsequent history (see Section 5.3) also limit transferability of sea-ice ecosystem models between different types of ice. Hence, it is important that biogeochemical sea-ice observations include explicit information on the location and as much insight as possible into the history of the ice.

Common data sheets can help create consistent observational data sets that include the necessary ancillary data. Several such sheets have been developed by the Antarctic Sea-ice Processes and Climate (ASPeCt) expert group and are available from the Australian Antarctic Data Centre (<http://data.aad.gov.au/aadc/seaice/>). These data forms include fields for general information about the sampling station and sea-ice environment, as well as detailed information on temperature, salinity, and the particular variables of interest, in consistent units and with common depth resolution. Even if it is not possible to fill out every column of the data template, the use of such a template greatly facilitates later observational data intercomparison and inclusion of the data in modelling efforts.

Finally, a note on units is required. Although it is best to use standardized units when reporting data, we acknowledge this issue to be a tricky one, as unit conversions must not involve unreasonable assumptions. Examples of inappropriate unit conversions include reporting data averaged over longer periods than the



measurements (e.g., using units month<sup>-1</sup> or year<sup>-1</sup> for gas fluxes only measured over a couple of days or weeks), and conversions between Chl<sub>a</sub>, cell numbers, and carbon content for mixed communities. Any assumptions used in averaging and upscaling the values always need to be stated, explicitly.

### 5.2. Fast ice versus pack ice

Currently, the available 1D sea-ice models do not consider biogeochemical differences between types of sea ice (i.e., fast versus pack ice, first-year versus multi-year ice). This is because to date, most of the models have been applied to coastal, landfast ice locations, because biogeochemical time series are available for this type of ice. While fast ice forms and melts in the same place, and thus the associated sympagic community can be considered typical of the area, pack ice is transported by winds and currents, and the associated biological community is not necessarily representative of the location where the ice was sampled (Garrison et al., 2005). In addition, fast ice is mostly undeformed and dominated by columnar ice, whereas pack ice can be very highly deformed and be a more complex mixture of columnar and granular ice, as well as gap layers, ridges, and keels.

Biological growth is mostly limited to the bottommost part of land-fast columnar ice, where higher temperatures and permeability allow exchange with the underlying waters. Hence, most 1D models include only one biological layer at the bottom, the thickness of which is either static (i.e., prescribed; Arrigo et al., 1993; Lavoie et al., 2005; Nishi and Tabeta, 2005; Jin et al., 2006) or dynamic (i.e., a function of permeability; Tedesco et al., 2010). However, deformation processes in pack ice (ridging and rafting) redistribute the biomass as well as nutrients within the sea-ice column (Horner et al., 1992; Gradinger et al., 2010; Meiners et al., 2012; Vancoppenolle et al., 2013b), and the potential for algal production higher up in pack ice, as well as the difference in permeability between granular and columnar ice, may be very important for gas exchange and aerosol production. Thus, the history of the ice may ultimately define exchange rates, yet there is no information available on how to model vertically distributed biomass. Ridged ice is particularly difficult to access and sample representatively, and therefore, is still severely undersampled. As we incorporate sea-ice biogeochemistry in 3D-numerical models (e.g., Deal et al., 2011; Dupont, 2012), the relationship between ice structure, which varies on large scales, and sea-ice biogeochemical processes needs to be quantified.

### 5.3. Arctic versus Antarctic sea ice

Many sea-ice ecosystem processes occurring on small scales are the same or at least similar in Arctic and Antarctic sea ice. However, there are some general differences in the formation and evolution and, therefore, structure of sea ice in the two regions (e.g., Spindler, 1990). The differences derive primarily from the fact that the Arctic Ocean is a relatively low-energy environment, surrounded by continents, with large, shallow continental shelves, while the Antarctic is a continent with large ice shelves surrounded by a relatively high-energy ocean exposed directly to global swell and fetch. As a result, Arctic sea ice has a more columnar structure, characteristic of formation in calmer waters, more multi-year ice (though the amount has decreased in recent years, e.g., Comiso, 2012) and more deformation dominated by ridging. Antarctic sea ice tends to be more granular, characteristic of formation in rougher waters or via snow-ice formation (flooding of snow by seawater, followed by refreezing), contains predominantly first-year ice, and deforms predominantly by rafting. Melt ponds and sedimentary materials are more common in Arctic ice, while Southern Ocean ice tends to have higher snow accumulation, causing surface flooding. Finally, the presence of large glacial ice shelves in the Antarctic leads to more frequent formation of platelet ice layers under the sea ice. These differences have implications for permeability and fluxes, as well as for sea-ice community distributions within the sea-ice column, and limit the application of individual sea-ice biogeochemical models to both the Arctic and Antarctic. In order to generate models with sound representation of the important processes at work in Arctic versus Antarctic sea ice, we need to better understand the variations due to ridging and rafting, the differences in permeability between granular and columnar ice, and the formation of frazil ice.

## 6. How to successfully collaborate and achieve maximum benefits

A modeller's wish list tends to include everything, preferably everywhere at every time. We acknowledge that this is not possible, but we think it is important to create a general list for an ideal model evaluation exercise and encourage observers to follow it within their logistical and funding constraints.

In short, ideal observations in support of sea-ice biogeochemical model development would be:

- 1) multidisciplinary, with physical, biological, and chemical properties measured at the same time and the same place to understand causes, effects, and feedbacks;
- 2) comprehensive, with all of the ecological domains (atmospheric, cryospheric, pelagic, and benthic) measured when possible, to link them and understand the fluxes between them;

- 3) spatially and temporally extensive, with long time series that span ice formation, ice melt, and the open water season, preferably over a reasonable spatial extent, to gain a holistic understanding; and
- 4) quantitative, as moving from conceptual to numerical models requires quantification of processes and rates.

The list tends to shorten considerably if modellers and observers work together from the onset of a program to focus on common hypotheses. In such a case, rather than asking how observations can improve models, such partnerships would be aiming at combining (even imperfect) models with (very restricted) measurements to improve our understanding of specific processes. All modellers and observers likely agree that sampling in polar regions is difficult, expensive, and consequently observations are sparse and heterogeneous. Hence, it is only logical to ask ourselves: How can we derive the most benefit from what measurements we can make?

Of course, ultimately any observations can usefully contribute to the development of better numerical models, as long as the results contribute to conceptual models of how the system works or the data can be merged with those from other studies to generate perspectives on temporal and spatial variability. However, ideal observations to support sea-ice biogeochemical model development would:

- 1) follow the best practices that have been established by the sea-ice community (e.g., Eicken et al., 2009; Miller et al., 2015);
- 2) use common measurement data templates (i.e., those available from <http://data.aad.gov.au/aadc/seaice/>);
- 3) establish and maintain coordinated databases (e.g., Meiners et al., 2012);
- 4) always provide ranges of uncertainty and detection limits;
- 5) use consistent units and provide the ancillary data necessary to convert between different units;
- 6) express species compositions in terms of organism function in the ecosystem (i.e., functional types), and fluxes in terms of meteorological, hydrological, and other physical conditions, while also clearly expressing the limitations of those extrapolations;
- 7) sample the entire depth of the ice and record depth-resolved observations.

To enhance successful collaboration, modellers need to acknowledge the hard work and expertise that goes into each data point and recognize the limitations of an observed data set, while observers should recognize models as tools that can:

- 1) support their results and provide a larger context;
- 2) extend their results beyond the limited area that was sampled;
- 3) produce improved understanding and new knowledge; and
- 4) support planning of more cost-effective expeditions and monitoring programs.

Conversely, to derive maximum benefit from the measurements, modellers need to: 1) specify their needs; 2) prioritize their needs; 3) discuss feasibility with the observers (material and time constraints, distance from laboratories, human resources, berth and laboratory space, etc.); and 4) accept feedback from observers and revisit prioritizations. In addition we would like to acknowledge that there are observations that do not directly feed into numerical models, but are valuable in this context nonetheless, contributing to the construction of the common conceptual model.

## 7. Summary

In this article, intended for scientists who are studying sea-ice biogeochemistry in the field and in laboratories, we have tried to provide a compilation of needs for sea-ice biogeochemical modelling on different temporal and spatial scales. Our aim has been to provide a better understanding of what kind of observations modellers need and, consequently, how field campaigns should be designed to support modelling efforts and how the results should be reported to help modellers get the most from the observations. We acknowledge that the dichotomy between observer and modeller is artificial, and a scientist studying sea-ice biogeochemistry can be (and ideally would be) both. Indeed, we encourage all polar observing scientists to keep numerical modelling in their toolboxes, and every modeller to get into the field as often as is practical.

Our common goal is to improve our understanding of the sea-ice ecosystem, its interactions with surrounding media, and its potentially large-scale effects. To achieve this goal we need to pool our resources, requiring funding agencies and research groups to join efforts and plan coordinated but cost-effective polar, multi-disciplinary campaigns. Frequent exchanges between the observational and modelling communities are important so that each party remains up-to-date on the other's needs and capabilities. There are valuable insights to be gained by combining modelling and observational expertise. Most collaborative efforts are initiated during workshops, where brainstorming is used as an efficient tool for developing synergies and address communication issues. We recommend, that organizers of workshops on the biogeochemistry of sea ice, systematically schedule timeslots for explicit discussions between modellers and observers. Planning field programs as part of larger, national or international network projects, which include both observers



Figure 4

A five star observer from a modeller's perspective.

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and modellers and have regular (annual or semi-annual) meetings where all participating groups present their tools, issues, and preliminary results, seems to be an effective way forward, even if not always feasible. In addition, new scientists entering this field should be encouraged to develop observational and modelling skills in parallel, and graduate student committees should include representatives from both communities.

Small experiments, both in the field and in laboratories, can be immensely useful, if they focus on a particular, critical question and the measurements follow appropriate community standards. In both large observational surveys and small-scale experiments, the willingness to learn and understand the needs and limitations of each collaborator's tools is a fundamental component of a successful collaboration.

We conclude that, from a modeller's perspective, a five-star observer is the one who measures a process of most interest repeatedly in several places and for long time periods and has a good global understanding of the variability that might drive the process being studied (Figure 4). We leave it to the observers to design a five star modeller.

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## Contributions

- NS wrote the first draft and coordinated and synthesized the contributions from the other authors.
- CD, DLan, DLav, SM, LM, LT, FM contributed text material, LT also contributed Table 2.
- EP contributed the idea for the cartoons.
- LM and JS ensured synthesis with observational scientists.
- All authors contributed to the evolution of the manuscript and provided comments at various stages.

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## Competing interests

No competing interests known

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