MARCHEMSPEC

Chemical Speciation Modelling in Seawater to Meet 21st Century Needs

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1 Summary

Trace elements are important in the world's oceans and near-shore environments as nutrients, tracers, and contaminants. The dissolution of anthropogenic CO_2, a component in the oceanic carbon cycle, is a cause of ocean acidification. Despite the importance of chemical speciation in these marine biogeochemical processes and their consequences for global change, the available models and other calculation tools – often based upon the Pitzer equations – are relatively fragmented and are usually restricted to particular chemical compositions and ranges of temperature and pressure. The models are often neither user-friendly nor freely available, and the community lacks a comprehensive evaluation that relates the capabilities of speciation models to current needs in chemical oceanography (e.g., programmes such as GEOTRACES). To address these problems we will review and document the current status, uncertainties, and basis in laboratory measurements of Pitzer models of seawater and complexation of trace metals (including micronutrients such as Fe, Cu, and Zn). We will define their current capabilities and limitations for oceanographic and biogeochemical calculations, and establish requirements for the future. We will consult widely and develop a specification for a set of speciation models and associated documentation that will be interactive and web-based. Making use of our previous very successful work in this area (and with external funding) we will create the website and associated tools. This requires a coordinated international effort, particularly to ensure that the modelling tools meet the needs of a wide range of potential users in both research and capacity building. A SCOR Working Group is the ideal mechanism for this development.

2 Background and Rationale

2.1 Speciation models and data

Chemical speciation is defined as the distribution of a chemical element between different molecular and ionic forms in seawater. It determines the reactivity and bioavailability of the elements in seawater, and is key to our understanding of biogeochemical and acidification processes in the ocean. It is necessary to model speciation in order to predict how the rate and extent of chemical reactions in the global ocean will be affected by increasing temperature and decreasing pH.

The form in which a trace element or other component of seawater is present, and its tendency to react, depends on its *activity* (Clegg and Whitfield, 1991). This is the product of its concentration (usually molality) and an activity coefficient (γ) which is a complex function of temperature, pressure, and salinity (or, more generally, solution composition). Many of the important reactions in seawater involve acid-base equilibria, which introduces pH as a further variable. Changing pH is also at the heart of the process and effects of CO_2 uptake by the oceans, and of the speciation of dissolved inorganic carbonate. The definitions of pH and the use of buffers to calibrate pH instruments, and the relationship of measured pH to that calculated using thermodynamic models of seawater, are complex and not always appreciated.

It is desirable to be able to calculate pH, and the activities and speciation of all seawater components, within a unified framework that, (i) includes the major and trace elements in seawater and its mixtures with freshwaters,

(ii) encompasses the buffers that are used to calibrate pH and other instruments, and (iii) can be extended to include other saline environments such as brines and pore waters. Progress has been made towards this goal, mainly in the 1980s and 1990s, and today the principal chemical speciation model of seawater is that of Millero and co-workers at the University of Miami (Waters and Millero, 2013, and references therein; see also Clegg and Whitfield, 1995). The model uses the equations of Pitzer (1991) to calculate activity coefficients, and is applicable primarily to major ion seawater (from 0 to 50 ^oC, and 0 to >40 salinity) containing the species H^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, Sr^{2+}, Cl^-, Br^-, OH^-, HCO_3^-, $B(OH)_4^-$, HSO_4^-, SO_4^{2-}, CO_3^{2-}, CO_2, $B(OH)_3$, and H_2O.

The measurements that are used to build models of mixtures such as seawater include: solvent and solute activities, apparent molar enthalpies and heat capacities (yielding the variation of the model parameters with temperature), apparent molar volumes (yielding the variation of the parameters with pressure), and other data. Complexation of trace metals by a number of ligands, both inorganic and organic, has been measured in artificial seawaters or simplified analogues (e.g., $NaCl_{(aq)}$), but usually over restricted ranges of concentration, at a single temperature (often 20 or 25 ^oC), and only at atmospheric pressure. The results often depend on the methods used to make the measurements.

The numbers of new studies yielding the activity, thermal, and volumetric data and stability constants needed to develop our quantitative understanding of speciation in the oceans have been in decline for many years, even as the need to model the biogeochemistry and especially the carbonate chemistry of the oceans has become greater. The numbers of skilled experimenters and modellers have also fallen. Furthermore, there is no comprehensive evaluation that relates the capabilities of speciation models, and the measurements upon which they are based, to current and future needs in chemical oceanography as exemplified in current programmes such as GEOTRACES. **Objective 1** of this working group is therefore to document the current status, and basis in laboratory measurements, of Pitzer models of seawater and estuarine water and the complexation of key trace metals including Fe, Cu, Mn, Cd, Mn, and Zn. We will define current capabilities and limitations for oceanographic and biogeochemical calculations, and establish what is needed (in both laboratory measurements and modelling) to meet future requirements. The associated **Objective 2** is to provide a database of Pitzer model parameters and equilibrium constants for seawater (and their variation with temperature and pressure), including trace metal complexation, which can be used by skilled practitioners. The uncertainties, and the effects on calculated properties such as pH, will be evaluated.

2.2 Applications in research and capacity building

The use of computer programs to carry out chemical speciation and other complex calculations for aqueous solutions and natural waters has traditionally involved obtaining the program from the authors, understanding input and output facilities intended only for the authors' use, and learning to use the program with few instructions. These obstacles have hampered the use of state-of-the-art models and the spread of best practice in modelling.

The world-wide-web is the ideal means of making modelling tools universally available for interactive use – with a variety of user interfaces suitable for the problems being solved and the skills of the user – and for providing the supporting information and tutorials needed by both researchers and students. For example the ecological modelling package ERSEM (European Regional Seas Ecosystem Model) has just been released as a freely available download to the marine science community (see http://www.shelfseasmodelling.org/) One of us (SLC) has over 15 years' experience providing chemical speciation and gas/liquid/solid equilibrium models that can be used *interactively* on the web (the Extended Aerosol Inorganics Model (*E-AIM*: http://www.aim.env.uea.ac.uk/aim/aim.php, see Wexler and Clegg, 2002). Usage statistics for *E-AIM* demonstrate the benefits for research and capacity building that universal availability and ease of use can bring: in 2013 more than 32,000 individually entered calculations were carried out by users around the world (38% from the Americas, 35% from Europe, and 24% from Asia).

We believe that a similar website, for chemical oceanography applications related to the carbonate system and to trace metal speciation, could bring even greater benefits. **Objective 3** is to develop a written specification for such a website, based upon consultation within the group and with other programmes. This will, for example, define the range of chemical systems and types of problems to which the speciation models will be applied (hence the design of the user interfaces and supporting "help" information), and requirements for capacity building (tutorials and demonstrations). Other modes of use will also be considered (e.g., calls from users' own program code; generation of lookup tables for use in large scale models). **Objective 4** is to create the fully-functioning website.

2.3 Why a SCOR working group?

The work that we propose cannot be driven solely by the modellers who are experts in their field. An in-depth understanding of the requirements of different potential user groups is essential. This will enable us to define the key equilibria and chemical species to be included, and give direction to the review of currently available data (on which current models are based). It will also enable us to specify the requirements for web-based modelling tools and associated training and teaching elements. SCOR, with its broad coverage and links to other international programmes, provides the ideal basis for developing a consensus across the global chemical oceanography community. The outputs of this Working Group will both stimulate new measurements of physico-chemical properties to better understand chemical speciation, and advance our ability to model speciation and its role in oceanographic and biogeochemical processes. The work that we propose, including its strongly international element, is rarely fundable by standard research grants from national research agencies. That is why we are approaching SCOR.

3 Terms of Reference

1) To document the current status, and basis in laboratory measurements, of Pitzer models of seawater and estuarine water focusing on the chemistry of ocean acidification and micronutrient trace metals (including, but not limited to, Fe, Cu, Mn, Cd, Mn, and Zn). Current capabilities and limitations for oceanographic and biogeochemical calculations will be defined, and future needs established. Important gaps in knowledge, which should have high priority for new measurements, will be

identified. The components to be covered will include the seawater electrolytes, the selected trace metals, and buffer solutions and key organic ligands such as those used in CLE-CSV titrations.

2) To publish the results of the first term of reference in the refereed scientific literature, and to introduce the conclusions and recommendations to the oceanographic community at a "town hall" event or special session at an international ocean sciences meeting.
3) To specify the functions and capability for a web-based modelling tool that will make chemical speciation calculations easily accessible for a wide range of applications in oceanography research and teaching, and thus improve understanding and spread best practice in modelling.
4) To implement the web-based tool for chemical speciation calculations, based upon the specification developed in the third term of reference which will also be used to obtain external funding to develop the programs, documentation, and site.

4 Work Plan

There are several parallel strands to the activities of the WG. The timetable is given below, after further details of the objectives.

In the review and database constituting **Objectives 1 and 2**, the range of physicochemical conditions to be covered will be those relevant to estuarine and oceanic waters: temperature -2°C to 40°C; salinity 0 to concentrated brines (but with a strong focus on salinity 35); pressure 1 to 1000 atmospheres. The matrix of Pitzer model parameters for a major ion seawater of the composition noted in section 2.1, even excluding Sr^{2+} and boric acid, is considerable: 40 sets of cation-anion interactions, and potentially 250 ternary or "mixture" parameters. Although some can be neglected where all the interacting species are at very low concentration, the large numbers of interactions and the fact that they can vary with both temperature and pressure in the oceans emphasises the need to: (1) assess the completeness of any model and its basis in measured thermodynamic properties, (2) carry out an uncertainty analysis for the calculated quantities, and (3) establish what further measurements are required to completely characterise the behaviour of the seawater/estuarine water for its major and minor components, and trace metals, for the ranges of conditions encountered at sites around the world.

Our survey will relate the modelling and data needs to current developments in marine biogeochemistry, including the consequences of climate change and other anthropogenic forcing functions. This assessment will result in a state-of-the-art, self-consistent, database. It will also identify knowledge gaps that limit our ability to complement current research programmes such as GEOTRACES, IMBER and SOLAS with relevant calculations of chemical speciation.

To attain **Objective 3** we will first review current calculation tools and programs, including their availability and use by oceanographers. These programs include Pitzer seawater and brine models, and those for specific problems such as *CO2SYS* for the inorganic carbonate system. We will define the scope of solution chemistry and speciation modelling to be implemented, the types of problems to which the speciation models will be applied (hence the design of the user interfaces and supporting "help" information), and requirements for capacity building (tutorials and demonstrations). We will develop the specification for the website and speciation tools, matched to the capabilities, needs, and levels of expertise of users. Consultation between members of the WG, and with other programmes, will feed into this.

In the final phase, for **Objective 4**, we will create a fully-functioning chemical speciation site for oceanographers. Experience with the *E-AIM* aerosol chemistry website, developed partly with external funding, shows that this will require specialist expertise in web implementation that is not available within the WG. We will therefore seek the additional resources necessary for this work, and work on the speciation models, during second year of the WG. In this phase the WG members will act as a test and advisory panel, and help ensure that the supporting information (help texts and training material) is sufficient and correct. Success (or otherwise) in the funding effort constitutes a decision point in the timetable, which is shown below.

Month 1: 1st full WG Meeting.

- This will focus on planning. Issues include: the seawater components and trace elements, and ranges of physicochemical conditions, to be covered (based upon user needs); the allocation of tasks; compilation of a list of external contacts for consultation (in other programmes); and plans for securing additional funding for the web development.

Months 2 - 11

- Objectives 1 & 2: Collection and review of relevant physico-chemical information for the seawater electrolyte; analyses of current Pitzer parameter databases for data sources and coverage of agreed systems and environmental conditions; uncertainty analysis.
- Objective 3: User representatives defining requirements for the web-based speciation tools in research and capacity building (including external consultations); drafting of a proposal for funding to develop the web-based speciation tools and site.

Month 12: WG Sub-group Meetings

- There will be two sub-group meetings: the first will discuss progress on the Pitzer parameter database, and the second will agree the basic specification of the web-based modelling tools sufficient for a draft proposal.

Months 13 - 23

- Objectives 1 and 2: Collect and review all relevant information for trace components, and for pressure effects. Individuals will work on their sections of the draft paper and database. Assembly and completion of the draft paper, delivery to internal reviewers.
- Objective 3: Further consultations with working group members and participants in other programmes to define requirements for the user interface(s) of the web-based calculation tools and for associated teaching (capacity building) materials.

- Objective 4: Submission of proposal(s) to support the development of the web-based tools.

Month 24: 2^{nd} full WG Meeting

- We will review the draft manuscripts of the chemical speciation review paper, and the Pitzer model database, in preparation for submission to a journal. This is also a **decision point** for the development of the web-based modelling tools: we will report on the results of efforts to secure funding, and future prospects. If we have been successful, the project will continue as indicated below. Otherwise, we will either request a postponement (to allow further time to obtain support), or end the WG with the publication of the review paper, Pitzer parameter database, and report defining the needs for web-based tools for speciation calculations. Thus, even if additional funds are not obtained, the WG will (i) produce products valuable for scientists in this field; (ii) establish needs and give direction to future research; (iii) document the tasks needed to complete a Web-based tool.

Months 25 - 47

- Objective 4: Development of the web-based modelling tools and supporting programs and website information, with internal testing and review by WG members and other individuals towards the end of this period.

Month 48: 3^{rd} and final full WG Meeting.

- Members will report on their experiences testing the web-based modelling tools, from both research and capacity-building perspectives. We will agree any necessary revisions, and changes will be made within 2 months of this meeting. The website will then be made public.

We will, where possible, organise WG meetings to coincide with relevant conferences so that the normal SCOR funding for three meetings can be stretched to four, and will explore the possibility of co-sponsorship by IAPSO and IUPAC.

5 Deliverables

1) A review paper, to be published in an international chemistry journal. This will include a statement of current speciation modelling capabilities, a survey of the available physico-chemical data for the major and minor chemical components (particularly related to chemical speciation and equilibria), and the identification of gaps and needs for future models and measurements. (Objective 1)
2) Accompanying the paper, a database listing the currently available Pitzer model parameters and equilibrium constants for seawater and trace components, their variations with temperature and pressure, and their origins in laboratory measurements (how they were obtained, uncertainties, and the references). (Objective 2)
3) Presentation of the results and conclusions of the review paper, for discussion and to stimulate new work, at a talk or special session on chemical speciation at an international ocean sciences meeting. (Objectives 1 and 2)

4) A report defining (a) the scope and specification of speciation modelling tools needed by chemical oceanographers for research and teaching (capacity building); (b) how these tools should be implemented on a website to meet the needs of different potential user groups. (Objective 3)
5) A public website, with associated programs and documentation, meeting the specification set out in (4). (Objective 4)
6) Presentation of the website and its capabilities at a “town hall” meeting at an international ocean sciences conference. (Objective 4)

6 Capacity Building

There is an urgent need for capacity building in chemical speciation modelling. For example, many national and international research programmes are focused on Ocean Acidification (OA). Chemical speciation modelling is essential to an understanding of the development and consequences of OA, yet access to state of the art chemical speciation modelling tools is effectively restricted to a small (and ageing) group of marine scientists who are active researchers in the area. This WG will address the need for capacity building – training, and providing practical tools – at several levels.

Our vision is that state of the art chemical speciation modelling should be easily available to all marine researchers and students, not just the select few who have active research projects in the area. This will be achieved by the development of a web-based modelling tool that builds on a published, consistent and quality-controlled Pitzer database. The active involvement of representatives of key user communities in the WG will ensure that the structure and function of the web tool is appropriate for both research and teaching. In the case of teaching, we already have experience in providing tutorials and instructional videos on the subject of solution thermodynamics. The web-based modelling tools, augmented by the teaching and training materials, will provide the route to the capacity building so urgently needed in this field.

The work and products of the WG will also help to stimulate future capacity building and research in chemical speciation modelling. Publication of the reviewed database and release of the web tool will focus attention its importance. This will encourage new research efforts in this area, and develop a younger generation of scientists who can maintain and develop the database and modelling tools.

Finally, it is anticipated that the identification of important knowledge gaps in the database will stimulate new research to fill those gaps. History suggests that this is more than an idle hope. A 1981 paper co-authored by two of us (Turner et al., 1981) that identified the dearth of data on the carbonate complexation of trace metals, did indeed stimulate new measurements that now provide the basis for our understanding of this phenomenon in the oceans.

7 Working Group Composition

The WG will have 10 Full Members with the range of expertise needed to address the terms of reference, including speciation modelling, large scale biogeochemical modelling, metal-ligand titration techniques, chemical-biological interactions and teaching. Importance is attached to ensuring that the modelling tools to be developed are readily accessible to the whole community, thus "users" are in a majority in the WG membership. They represent a broad geographical spread, from Europe, North America, South America, China and New Zealand. Although the applications are not restricted to **GEOTRACES**, we see this project as an important complement to **GEOTRACES** that lies outside that programme's field focus. The Full Members include four members of the **GEOTRACES** SSC (Turner, Hatje, Maldonado, Tagliabue), which will ensure effective coordination. The Associate Members provide additional complementary user expertise, together with experienced modellers (including 2 members of the related SCOR WG 127, see section 9.4) who can contribute to reviewing the database and model development.

7.1 Full members

Name	Gender	Place of Work	Expertise
David Turner (chair)	M	University of Gothenburg, Sweden	Physical chemist, oceanographer and modeller: chemical speciation in seawater
Simon Clegg (vice-chair)	M	University of East Anglia, UK	Modeller: chemical thermodynamic modelling (inc. Pitzer equations), development of web-based tools for research and teaching
Sylvia Sander (vice-chair)	F	University of Otago, New Zealand	User: experimental studies of trace metal speciation, focus on data analysis
Heather Benway	F	Woods Hole Oceanographic Institution, USA	Executive Officer, Ocean Carbon and Biogeochemistry Project Office; expert in communication and outreach.
Arthur Chen	M	National Sun Yat-sen University, Taiwan	User: CO_2 system, estuarine, and marine and hydrothermal biogeochemistry
Andrew Dickson	M	Scripps Institute of Oceanography, USA	Physical chemist and modeller: CO_2 system in seawater, reference materials for measurements
Vanessa Hatje	F	INCT Energy and Environment, Bahia, Brazil	User: trace metal accumulation in marine organisms
Maite Maldonado	F	University of British Columbia, Canada	User: biological oceanographer
Alessandro Tagliabue	M	University of Liverpool, UK	User: development of global biogeochemical models
Rodrigo Torres	M	Centre for the Investigation of the Patagonian Ecosystem (CIEP) , Chile	User: ocean acidification and iron

7.2 Associate members

Name	Gender	Place of Work	Expertise
Eric Achterberg	M	GEOMAR, Kiel, Germany	User: chemical oceanographer, CO_2 system and trace metals
Yuri Artioli	M	Plymouth Marine Laboratory, UK	User: ecosystem modeller, member of the ERSEM group
Giles Marion	M	Desert Research Institute, USA	Modeller: developed the FREZCHEM chemical speciation model for cold water systems (http://frezchem.dri.edu/main.html)
Peter May	M	Murdoch University, Australia	Physical chemist and modeller, author of Joint Expert Speciation System (JESS).
Frank Millero	M	University of Miami, USA	Physical chemist and modeller: many measurements of the thermodynamic properties of seawater, and long experience of applying Pitzer models to marine systems
Stan van den Berg	M	University of Liverpool, UK	User: competitive ligand titrations in seawater
Wolfgang Voigt	M	TU Bergakademie Freiberg, Germany	Physical chemist and modeller: properties of concentrated salt solutions and brines (THEREDA database). May also involve close colleague Helge Moog.
Christophe Völker	M	Alfred Wegener Institute, Germany	User: development of global biogeochemical models
Dewen Zeng	M	Institute of Salt Lakes, China	Physical chemist and modeller: expert in chemical speciation with a background in hydrometallurgy.

8 Working Group Contributions

David Turner contributes a broad-based understanding of the field, with experience in chemical speciation modelling, and also in field-based biogeochemistry as Chief Scientist on 3 JGOFS cruises. He also contributes experience as a former WG co-chair (WG109, co-sponsored with IUPAC).

Simon Clegg (modeller) has long experience in applying Pitzer equations both to seawater and atmospheric aerosols, and has an extensive knowledge of the data upon which they are based. His experience in developing the *E-AIM* modelling website (section 2.2) will also make an important contribution to the WG.

Sylvia Sander (user) is expert in competitive ligand titrations, which are used to characterize metal-organic binding in seawater: there is a clear need for improved speciation modelling in this area. As one of the leaders of WG139, she will be able to ensure that the two WG:s complement each other effectively.

Heather Benway (capacity building) is an essential link to the Ocean Carbon and Biogeochemistry Programme, for which she is Executive Officer. She also brings a strong record of outreach and community involvement and will contribute greatly to the teaching and training elements of the web-based speciation tools.

Arthur Chen (user) contributes a wide expertise in marine, estuarine and hydrothermal biogeochemistry and the application of speciation modelling to these systems.

Andrew Dickson (modeller) is an expert in laboratory measurement and modelling of chemical speciation; and also in the development of standard materials, calculation methods and documentation for the marine CO_2 system.

Vanessa Hatje (user) contributes expertise in the study of the trace metal content of marine organisms, an area where improved chemical speciation modelling is needed.

Maite Maldonado (user) contributes expertise in the study of chemical-biological interactions, most particularly the uptake of trace metals by microorganisms. Understanding uptake processes is dependent on good chemical speciation models.

Alessandro Tagliabue (user) contributes expertise in global biogeochemical modelling where there is a clear need for improved descriptions of (particularly) iron speciation.

Rodrigo Torres (user) contributes expertise in studies of ocean acidification and its consequences for iron biogeochemistry

9 Relationships to Other Programmes and SCOR Working Groups

9.1 GEOTRACES

The data generated by the **GEOTRACES** programme, as exemplified by the recently released Intermediate Data Product, is a game-changer in marine biogeochemistry. **GEOTRACES** involves simultaneous sampling for key trace elements and supporting parameters with an accuracy, coverage and resolution far beyond that previously available for trace elements. However, the marine biogeochemistry community currently lacks readily available tools for complementing the **GEOTRACES** data with state of the art calculations of chemical speciation. This proposal aims to fill that gap.

9.2 Global change programmes

The need to understand the effects of climate change and other anthropogenic forcings on marine biogeochemistry is inherent in a number of international programmes such as **IMBER** and **SOLAS**, large scale models such as the **European Regional Seas Ecosystem Model**, and national programs such as the Ocean Acidification Programme in the UK (**UKOARP**, see below). This will continue as a priority within the Future Earth programme now under development. Within these programmes there is an increasing focus on multi-stressors, i.e. the way in which different forcings combine synergistically or antagonistically to produce a net effect. An understanding of chemical speciation is of key importance here. Iron, which is now known to be a limiting nutrient in large areas of the ocean, is one example. The proposed WG is highly relevant to these ongoing and future studies.

9.3 UK national programmes

Both the **UKOARP** and the Shelf Sea Biogeochemistry Programme (**SSB**) have been contacted, and common interests identified. A UK-hosted workshop in 2015 is likely to be attractive to **SSB**, and co-funding is possible. This will be requested later in 2014 when the announcement of opportunity for such 'added value activities' is made.

9.4 SCOR WG 127

The thermodynamic equation of state for seawater, 2010, was produced by this WG. It is a Gibbs function (an equation) from which the thermodynamic properties of seawater are calculated. Most relevant to this WG is the fact that the osmotic coefficient, and also the density, of seawater can be calculated from TEOS 2010. These are important constraints for the speciation models, and should be adhered to.

9.5 SCOR WG 139

The current SCOR WG, entitled "Organic Ligands – A Key Control on Trace Metal Biogeochemistry in the Ocean", addresses the experimental characterisation of interactions between trace metals and natural organic matter in the ocean. There is a strong focus on the use of competitive ligand titrations, from which stability constants and concentrations are derived for a small number of "ligands". Our proposal complements WG 139 by providing (i) a chemical speciation model for all other interactions affecting the trace metal in question; (ii) a chemical speciation model for the titrations that are frequently used to characterise the trace metal – natural organic interactions; and (iii) a framework for including the experimentally derived "ligand" concentrations and stability constants in a chemical speciation model. The leadership of WG 139 has confirmed that this proposal does not overlap WG139.

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S. L. Clegg and M. Whitfield (1995) A chemical model of seawater including dissolved ammonia, and the stoichiometric dissociation constant of ammonia in estuarine water and seawater from -2^{o} to 40^{o}C. *Geochim. et Cosmochim. Acta* **59**, 2403-2421.

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A. S. Wexler and S. L. Clegg (2002) Atmospheric aerosol models for systems including the ions H^+, NH_4^+, Na^+, SO_4^{2-}, NO_3^-, Cl^-, Br^-, and H_2O. *J. Geophys. Res.-Atmos.* **107**, D14, Art. No. 4207.

Appendix: Key Publications of Full Members

David Turner

(1) Z. Abbas, A. Ulfsbo and **D.R. Turner** (2013) Monte Carlo simulation of the dissociation constants of CO_2 in 0 to 1 molal sodium chloride between 0 and 25 degrees C. *Mar. Chem.* 150, 1-10.

(2) E. Breitbarth, J.Gelting, J. Walve, L.J. Hoffmann, **D.R. Turner**, M. Hassellöv and J. Ingri (2009). Dissolved iron (II) in the Baltic Sea surface water and implications for cyanobacterial bloom development. *Biogeosciences* **6**, 2397-2420.

(3) P.L. Croot, K. Andersson, M. Öztürk and **D.R. Turner** (2004). The distribution and speciation of iron along 6°E in the Southern Ocean. *Deep-Sea Res. II* **51**, 2857-2879

(4) **D.R. Turner** and K.A. Hunter, eds (2001). *The Biogeochemistry of Iron in Seawater*. 2001, John Wiley, Chichester, 396pp

(5) **D.R. Turner**, M. Whitfield, and A.G. Dickson (1981). The equilibrium speciation of dissolved components in freshwater and seawater at 25°C and 1 atmosphere pressure. *Geochim. Cosmochim. Acta*, **45**, 855-881.

Simon Clegg:

(1) C. S. Dutcher, X. Ge, A. S. Wexler, and **S. L. Clegg** (2013) An isotherm-based thermodynamic model of multicomponent aqueous solutions, applicable over the entire concentration range. *J. Phys. Chem. A.* **117**, 3198-3213.

(2) **S. L. Clegg** and A. S. Wexler (2011) Densities and apparent molar volumes of atmospherically important electrolyte solutions. 2. The systems H^+-HSO_4^--SO_4^{2-}-H_2O from 0 to 3 mol kg^{-1} as a function of temperature and H^+-NH_4^+-HSO_4^--SO_4^{2-}-H_2O from 0 to 6 mol kg^{-1} at 25 °C using a Pitzer ion interaction model, and NH_4HSO_4-H_2O and $(NH_4)_3H(SO_4)_2$-H_2O over the entire concentration range. *J. Phys. Chem. A* **115**, 3461-3474.

(3) **S. L. Clegg** and J. H. Seinfeld (2006) Thermodynamic models of aqueous solutions containing inorganic electrolytes and dicarboxylic acids at 298.15 K. II. Systems including dissociation. *J. Phys. Chem. A* **110**, 5718-5734.

(4) A. S. Wexler and S. L. Clegg (2002) Atmospheric aerosol models for systems including the ions H^+, NH_4^+, Na^+, SO_4^{2-}, NO_3^-, Cl^-, Br^-, and H_2O. *J. Geophys. Res.-Atmos.* **107**, D14, Art. No. 4207. (*Extended Aerosol Inorganics Model*: http://www.aim.env.uea.ac.uk/aim/aim.php)

(5) **S. L. Clegg** and M. Whitfield (1995) A chemical model of seawater including dissolved ammonia, and the stoichiometric dissociation constant of ammonia in estuarine water and seawater from -2° to 40°C. *Geochim. et Cosmochim. Acta* **59**, 2403-2421.

Sylvia Sander

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SCOR Working Group Proposal

Title: Towards comparability of global oceanic nutrient data

Acronym: COMPONUT

Summary/Abstract (max. 250 words/246)

To better manage the global impacts of human activities on the world's oceans, it is necessary to have accurate observations of changes in carbon and dissolved nutrients in both upper and deep ocean waters. By establishing mechanisms for comparability of nutrient analyses, we will be able to detect changes in nutrient levels due to human impact and shifting physical processes. Such changes could, either alter the supply of nutrients to the upper ocean directly or be from changes to ocean circulation. A recent Framework of Ocean Observing statement introduced the concept of Essential Ocean Variables (EOVs), and the assessment and development of readiness for sustained observations, with the aim of promoting collaboration in developing requirements, observing networks, and data information streams. Nutrients are identified as one of these EOVs. In 2014, two certified reference materials (CRMs) will become available for measurements of nutrients in seawater; a CRM provided by the National Metrology Institute, Japan, and MOOS-3, provided by National Research Council, Canada. The whole situation now calls for further international collaboration through SCOR, with a Working Group to establish the mechanisms for comparable oceanic nutrient data, using globally accepted CRMs. The primary goal is that for nutrient data collected anywhere by one individual laboratory, and data collected over long time periods by one or more laboratories, will be consistent and traceable with certified comparability. For future generations it is unacceptable to produce historical data sets without the absolute consistency necessary to assess spatial and temporal trends.

Scientific Background and Rationale (max 1250 words/1248)

Changes are occurring on a global scale in ocean biogeochemical cycles and much of the cause of these changes, directly or indirectly, is from human activities. Therefore, it is necessary to have accurate observations of trends in carbon and dissolved nutrients in both upper and deep ocean waters. For these observations, it is critical that we can reliably compare results from different laboratories, for geographically similar ocean waters with total confidence. To get a global consensus for nutrient data, it is necessary to both have accepted certified reference materials (CRMs) and to have the requirement to use the CRMs, and these can be established by the authority of a SCOR Working Group. The focus for this proposed Working Group is for oceanic waters, but because the ranges of nutrients expected are similar, the effort can be extended, at least partially, to coastal and estuarine waters. There are currently established certified standardizations for only a few marine parameters; such as; temperature measurements (ITS90, traceable to SI using Standard Platinum Resistance Thermometer, SPRT), salinity measurements (comparability ensured using IAPSO salinity standard seawater provided by OSI, UK), and the carbonate system parameter measurements (comparability and traceability ensured using CRMs provided by Dickson's laboratory, SIO, USA, Dickson, 2003; 2010).

The 2007 IPCC Report highlighted the problem inherent in comparing data sets stating that: "Uncertainties in deep ocean nutrient observations may be responsible for the lack of coherence in the nutrient changes. Sources of inaccuracy include the limited number of observations and the lack of compatibility between measurements from different laboratories at different times" (Bindoff et al., 2007). Results of nutrient concentrations from global crossover station analysis have shown discrepancies of up to 10 % for deep nutrient data during the last three decades (Aoyama et al., 2013), and the results of inter-laboratory comparison studies since 2003 showed a similar magnitude of discrepancy among some participant laboratories (Aoyama et al., 2007; 2008; 2010). This indicates that analytical problems may cause larger discrepancies for deep water nutrients, and these reported comparisons were from a small number of specific studies, whereas there are many oceanic nutrient data sets reported, published, and stored on international databases, with no references to CRMs at all. Although this situation has been improved somewhat, it is still difficult to ascertain with any certainty temporal changes in ocean nutrients. We can now detect changes in deep ocean temperature (and hence heat content) (Levitus et al., 2009; 2012; Kouketsu et al. 2009; Rhein et al., 2013) from observations due to comparability of temperature measurements, on the order of mK. Changes to the carbonate system parameters in the deep ocean are also reported with comparability being ensured by the use of CRMs (e.g. Wanninkhof et al., 2010, Ríos et al., 2012, Khatiwala et al., 2012). Similarly, changes to oceanic oxygen can now also be accurately observed (Stendardo and Gruber, 2012).

It is important to now establish mechanisms for improving the quality of reported oceanic nutrient data, which will then allow us to be able to more accurately detect changes in nutrient levels due to human impact and shifting physical processes, which might alter the supply of nutrients to the upper ocean in the future. Improved comparability of reported nutrient concentrations in the water column will also help us to improve estimates of the anthropogenic portion of the observed increase of total carbon in the water column.

To properly guarantee comparability of data from different laboratories, the precise mechanisms of a global consensus for reporting nutrient levels needs to be established. This will foster a move toward the comparability of nutrient data using globally accepted RMs/CRMs, followed by the recommendation of protocols for their use throughout the world-wide marine chemistry community. This has already been achieved by the use of CRMs for measurements of the CO_2 system, and the use of the IAPSO standard seawater for salinity measurements. A potential problem with using nutrient CRMs is similar to that with the use of references for dissolved organic carbon (DOC); that is, some form of enforcement for their use should be established. There was significant improvement in community DOC measurement during the international JGOFS program due to encouragement by the US National Science Foundation and NOAA to participate in DOC comparability exercises (Sharp et al, 2002). A nutrient CRM SCOR working group should be able to provide the authority for not only certification of nutrient CRMs, but also for their use.

Historically, a U.S. National Research Council report (Dickson et al., 2002) clearly stated that certain key oceanic parameters lacked reliable and readily available reference materials. That report identified the most urgently required chemical reference materials based on certain key themes for oceanographic research. At the top of the list of the new reference materials needed were standards for the measurement of nutrients, with the statement: “There is an urgent need for a certified reference material for nutrients. Completed global surveys already suffer from the lack of previously available standards, and the success of future surveys as well as the development of instruments capable of remote time-series measurements will rest on the availability and use of good nutrient reference materials”. Since that time, RMs/CRMs for oceanographic use have been developed. These include a Danish RM, NRC-Canada CRM (MOOS-3), and one developed by KANSO-Japan. In 2014 NMIJ will start to provide CRMs (NMIJ CRM 7601-a, NMIJ CRM 7602-a, and NMIJ CRM 7603-a) with nutrient concentrations appropriate for the nutrient concentration ranges of Nitrate, Nitrite, Silicate and Phosphate found in the Pacific and Atlantic Oceans. MOOS-3 covers nutrient concentrations specifically for the Atlantic Ocean. Therefore, we now have the opportunity for traceability and comparability of nutrient concentrations throughout the globe, and a mechanism to provide RMs which is traceable to SI through CRMs. Global availability of the RM to traceable to NMIJ CRM will be made through JAMSTEC (Japan Agency for Marine-Earth Science and Technology), in a similar manner to the carbonate system CRMs from Dickson’s laboratory (SIO, Scripps).

A nutrient CRM calls for further international collaboration through SCOR, and a Working Group to establish the mechanisms required to provide comparability of oceanic nutrient data, using globally accepted RMs/CRMs. A major challenge with this SCOR WG is to develop a system by which the comparability of data within and between laboratories is better than 1% at full scale of nitrate, phosphate and silicate concentrations. The levels of comparability achieved for the measurement of oceanic salinity and total inorganic carbon are considerably better than 1%. However, both of those parameters are comparatively simple, chemically, and exist in the open ocean in much narrower concentration ranges than do the inorganic nutrients.

The primary goal for the SCOR Working Group is for nutrient data collected at any one place by an individual laboratory and data collected over long time periods by one or more laboratories to be consistent with certified comparability. The experience of this SCOR WG will also give positive feed-back to the scientific community of coastal ocean observatories, and for researchers developing nutrient sensors for buoys and floats, by providing and recommending globally accepted RMs/CRMs for the calibration of instruments and sensors. Such feedback will move toward the goal of achieving comparability of nutrient data throughout the oceans, which will have been obtained by different methods, instruments, and technologies. This initiative will be based on previously developed collaboration with the IOC-ICES SGONS that ended in 2012. For future generations it is unacceptable to produce historical data sets without the absolute consistency necessary to assess spatial and temporal trends.

Terms of Reference (max. 250 words/177)

1. To establish mechanisms to ensure comparability of oceanic nutrient data
2. To assess the homogeneity and stability of currently available RMs/CRMs. It remains to determine whether the current producers are achieving a level of precision within and between laboratories which is comparable to or better than 1 %.
3. To develop standardized data-handling procedures with common data vocabularies and formats, across producers and users, and will include the future linking of national and international data archives. The group will seek to involve international data center representatives to contribute to and lead this task.
4. To promote the wider global use of RM's by arranging workshops to actively encourage their use and to provide training in analytical protocols and best practice, particularly targeted towards developing countries.
5. To continue regular global inter-comparison studies, following on from the previous exercises in 2003, 2006, 2008 and 2012, with collaboration of IOCCP-SSG and RCGC-JAMSTEC.
6. To update the GO-SHIP nutrient measurement manual, which was originally a product of the IOC-ICES SGONS, (Study Group on Nutrient Standards).
7. To publish reports on this WG's activities and workshops.

Working plan (logical sequence of steps to fulfil terms of reference, with timeline. Max. 1000 words/446)

This Working Group will work 3 years after acceptance by the SCOR General assembly in 2014. The time-line shown below highlights only the main meetings/activities. We will have regular e-mail exchanges, Skype meetings, and a variety of workshops/meetings among the full and associated members that will occur on a regular basis.

Year 1: 2015

Kick-off Meeting: Upon funding, the WG will have a kick-off meeting in early to mid 2015. In order to provide good international visibility, the 2015 EGU General Assembly (April 12-17 2015, Vienna, Austria) is a good potential venue where a WG meeting #1 on changes of nutrients in the world's oceans and use of RMs/CRMs could be held.

Conduct an inter-laboratory comparison experiment of currently available RMs/CRMs by several selected key laboratories to assess the homogeneity and stability of currently available RMs/CRMs. This will be organized by a few of full/associate members of the WG. The results of this will be published as soon as possible after the experiment.

Year 2: 2016

A potential venue for the half-way meeting, WG meeting #2 will be the 2016 Ocean Sciences

Meeting (21 February 2016 — 26 February 2016, New Orleans, Louisiana, USA). During the OSM 2016, we will propose a presentation session at the meeting, and we will also hold a workshop to promote the wider global use of RM's, to actively encourage their use. We will also review synthesis papers and previously published inter laboratory comparison study reports, and prepare a revised version of the GO-SHIP nutrients measurement manual during this workshop. One of key issues is to update/confirm basic analytical methodologies for nitrate, nitrite, phosphate and silicate.

We will conduct a global inter-comparison study of RMs/CRMs following on from the previous exercises in 2003, 2006, 2008, 2012 and 2014, with the collaboration of IOCCP-SSG and RCGC-JAMSTEC.

In 2016 we will provide a training course in analytical methodologies and best practice of nutrient measurement, particularly for developing countries. Potential venues for this training course are NIOZ/The Netherlands, SIO/USA, or JAMSTEC/Japan. In this training course, participants will be given training by experienced analysts and the workshop will discuss the results of the global inter-comparison studies of RMs/CRMs so as to learn more about how to ensure comparability of oceanic nutrient data.

These opportunities, the training course and global inter-comparison study, will also contribute to building capacities in developing countries to measure nutrient concentrations in seawater.

Year 3: 2017

We will plan an international symposium "Towards comparability of global oceanic nutrient data". This symposium is also WG meeting #3. Potential venues for this symposium are JAMSTEC/Japan, NIOZ/The Netherlands and SIO/USA. We will particularly focus on inviting scientists from developing countries, and encourage their involvement in this symposium.

Deliverables (state clearly what products the WG will generate. Should relate to the terms of reference. Max 250/163). A workshop is not a deliverable. Please note that SCOR prefers that publications be in open-access journals.

1. Assessment reports of currently available RMs/CRMs based on inter-laboratory comparison experiments which will be submitted to 'Biogeochemistry' or similar open access journal.

2. A "best practice" manual which will provide the community with a recommended consistent approach to the sampling, analysis, use of RM's, quality control of nutrients, and subsequent data handling which will be an update of the GO-SHIP nutrients manual (Hydes et al 2010).

This manual will be available freely at the GO-SHIP website and will be able to be downloaded free of charge. A printed version of this manual may be published depending on additional funding availability.

3. A report on global inter-comparison studies of RMs/CRMs will be submitted to the journal "Earth System Science Data" published by EGU.

4. Synthesis papers on current nutrient measurements techniques/methodologies which will be submitted to the journal "Earth System Science Data" published by EGU.

5. A book will be published from the final International symposium "Towards comparability of global oceanic nutrient data".

Capacity Building (How will this WG build long-lasting capacity for practicing and understanding this area of marine science globally.Max500/277

This important aspect is reflected in two ways. The first is to promote participation of developing countries in inter-laboratory comparison studies of RM's through the involvement and help of POGO. The second is to invite participating laboratories to a 3-day training course in 2016 planned to be held at JAMSTEC/Japan, NIOZ/The Netherlands or SIO/USA (depending on additional funding) to learn more about analytical methodologies, best practice, and to discuss and interpret results of the global inter-laboratory comparison studies of RM's.

Building capacities in developing countries can be accelerated by providing a good simple manual based on "best practices" and we will encourage even greater participation in the future inter-laboratory comparison study of RM's proposed for 2016 from these developing countries. The aspect of capacity building could be further augmented by hosting a session (in conjunction with a WG meeting/AGU meeting/OSM meeting), at approximately mid-term, to discuss the needs and capabilities of developing countries with respect to using other suitable programs. We will initially instigate a targeted questionnaire to laboratories in developing countries to highlight their most important analytical requirements, this will all be accomplished with the help and advice of POGO.

The laboratories that took part in the 2012 inter-comparison exercise of nutrients in seawater are already from the following countries: Argentina, Australia, Belgium, Bermuda, Brazil, Canada, Cape Verde, Chile, China, Denmark, France, Germany, Iceland, India, Israel, Italy, Japan, Netherlands, New Zealand, Norway, Russia, Saudi Arabia, South Africa, South Korea, Spain, UK, USA, Venezuela. This proposed SCOR WG will endeavor to expand the global participation of developing countries from the current number of 2012/2014 representatives into the 2016 inter-calibration exercise with more participants from developing countries..

Working Group composition (as table). Divide by Full Members (10 people) and Associate Members, taking note of scientific discipline spread, geographical spread, and gender balance. (max. 500 words)

Full Members (no more than 10, please identify chair(s))

Name	Gender	Place of work	Expertise relevant to proposal
1 Michio Aoyama*	Male	RCGC-JAMSTEC/IER-Fukushima Univ., Japan	Geochemistry, global nutrients distribution
2 E. Malcolm S. Woodward*	Male	PML, UK	Nanomolar level precision measurements
3 Toste Tanhua	Male	GEOMAR, Germany,	Chairman of the International Ocean Carbon Coordination Project (IOCCP)
4 Karin Bjorkman	Female	Laboratory for Microbial Oceanography, Hawaii, USA	HOT time series
5 Bernadette Sloyan	Female	CSIRO, Australia	Co-chair of The Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP)
6 Anne Daniel	Female	IFREMER, France	French nutrient reference laboratory (DYNECO/PELAGOS, IFREMER
7 Susan Becker,	Female	SIO, USA	Repeat Hydrography
8 M. Dileep Kumar	Male	NIO, India	Chemical Oceanography
9 Claire Mahaffey	Female	University of Liverpool, UK	Nutrient Biogeochemist
10 Howard Waldron	Male	University of CapeTown, South Africa	Nitrogen dynamics in Ocean systems

* : Co-Chairs

Associate Member (no more than 10)

Name	Gender	Place of work	Expertise relevant to proposal
1 Alex Kozyr	Male	CIDIAC, USA	Multiple user database access
2 Karel Bakker	Male	NIOZ, The Netherlands	The Netherlands sea-going analytical facility
3 Takeshi Yoshimura	Male	CRIEPI, Japan	Organic Nutrients
4 Jonathan Sharp	Male	University of Delaware, USA	DOC RM experience
5 Andrew Dickson	Male	SIO, USA	Carbonate system RM experiences
6 Minhan Dai	Male	Xiamen University, China	Large global (LOICZ and Chinese programs)
7 Akihiko Murata	Male	JAMSTEC, Japan	Chemical oceanography, Global carbon/nutrient stoichiometry
8 Trevor Platt	Male	PKL, UK	Executive Director, POGO
9 Ralph Sturgeon	Male	NRC, Canada	CRM producer
10 Akiharu Hioki	Male	NMIJ, Japan	CRM producer

Working Group contributions (Max 500/500)

Michio AOYAMA organized the previous 4 Inter-laboratory comparison experiments for Reference Materials of Nutrients in Seawater, RMNS, in 2003, 2006, 2008 and 2012. He is working to develop RMNS, and has been PI of nutrients of 6 CLIVAR cruises in the Pacific Ocean. He is one of PIs of dissolve oxygen and nutrients part of Pacific Ocean Interior Carbon Data Synthesis project, PACIFICA. He has 104 publications in peer-reviewed journals and numerous reports.

Malcolm WOODWARD has worked as a Chemical Oceanographer for 35 years, and Head of the Plymouth Marine Laboratory Nutrients Facility for the past 20 years, has 100 publications in peer-reviewed journals and numerous reports. Has specialized and developed nanomolar nutrient analysis techniques and their applications in global oligotrophic oceans.

Toste TANHUA works on research fields of transient tracers in the ocean, ocean ventilation and mixing, tracer release experiments to quantify mixing. He also conducts CARINA Data Synthesis Project in the Atlantic Ocean. Now he works as a chair of The International Ocean Carbon Coordination Project (IOCCP). He has numerous publications in peer-reviewed journals reports and books.

Karin BJORKMAN works the field of microbial oceanography and nutrient dynamics with a special focus on phosphorus cycling in the oligotrophic North Pacific subtropical gyre. This work includes high sensitivity measurements low nano-molar concentrations of inorganic phosphate as well as the use of radioisotopes as tracers.

Bernadette SLOYAN works on International repeat hydrography and carbon program. She analyzes repeat hydrographic sections in the southern hemisphere oceans and simulation of deep ocean changes in climate models. She has numerous publications in peer-reviewed journals reports and books.

Anne DANIEL is in charge of the French reference laboratory (DYNECO/PELAGOS, IFREMER) for chemical measurement in marine and fresh waters. It supports laboratories by developing new methodologies, organizing performance tests and implementing quality system for accreditation according to the ISO/IEC 17025 norm. She also works in the implementation of the EU Water Framework Directive (WFD) and EU Marine Water Framework Directive (MSFD).

Susan BECKER is a manager and supervisor for the Oceanographic Data Facility within Shipboard Technical Support at Scripps Institution of Oceanography. She is responsible for overseeing the analytical analysis and data quality of inorganic nutrients, dissolved oxygen, and salinity. ODF provides the highest quality hydrographic data from CTD casts and discreet analysis of salinity, nutrients and dissolved oxygen for global repeat hydrography programs.

M. Dileep KUMAR is a Chemical Oceanographer focusing on nutrient and carbon biogeochemistry with particular reference to Climate Change. He has about 35 years of research experience at NIO (Goa) and has about 65 publications in peer-reviewed journals.

Claire Mahaffey is a nutrient biogeochemist and Senior Lecturer with over 10 years experience studying the source, cycling and fate of nitrogen, phosphorus and carbon in the subtropical open ocean and coastal and shelf seas. Has been responsible for nutrient analysis both at the Hawaii Ocean Time Series (USA) and Liverpool Bay Coastal Observatory (UK).

Howard WALDRON works on nitrogen dynamics of ocean systems including Benguela Upwelling, Southern Ocean and Atlantic Meridional Transect.

Relationship to other International programs and SCOR Working groups (max. 500 words/78)

Toste Tanhua is a Chair of The International Ocean Carbon Coordination Project (IOCCP).

Bernadette Sloyan is a Co-chair of The Global Ocean Ship-based Hydrographic Investigations Program (GO-SHIP).

Trevor Platt is an Executive Director of the Partnership for Observation of the Global Oceans

(POGO).

Michio Aoyama is a candidate of full member of SCOR WG proposal of marine radioactivity which will be submitted in 2014. Minhan Dai is also a candidate of co-chair of SCOR WG proposal of marine radioactivity.

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Appendix

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INSHORE: Proposal for a SCOR Working Group to form the International Network for the Study of How Organisms Respond to Environmental change

Abstract

Climate change and ocean acidification currently lead the international research agenda for marine ecosystems. Increased awareness of the effects of additional pressures arising from human activities has also led to the emergent research priority of 'multiple stressors', a theme recognized within international policy requirements for assessments of impacts on marine biodiversity. Despite increased understanding that global scale drivers will interact in complex ways with regional to local scale stressors to affect marine ecosystems, most research programmes currently study stressors in isolation. The effects of climate change are likely to be more complex than suggested by the simple trends and averages presently recognised. Similarly, most ocean acidification research has focused on single species mesocosms or small-scale observational studies across unrealistically short timeframes. A more realistic understanding of long term ecological responses to environmental change and multiple stressors requires a multidisciplinary organisms-to-ecosystems approach.

The overarching objective of the INSHORE Working Group is to develop a standard, integrative framework and modelling tool that can be applied internationally for research into multiple stressor impacts on coastal marine ecosystems. This will be achieved by 1) creating a global database of relevant ecological, biological and environmental datasets 2) developing a multiple stressor dynamic biostressor envelope model framework capable of operating over a range of spatial and temporal scales, 3) publishing a methodological best practice guide 4) hosting targeted workshops and a themed session at an international conference to engage the coastal benthic research community in an integrated scientific approach.

Scientific Background and Rationale

Scientific Background

Global climate change is now the milieu within which all biological, ecological and socio-ecological interactions must be positioned. The importance of a quantitative understanding of biological and physiological impacts of global change, and resultant changes to distributions and abundances of species within the marine environment is clear[1,2], with an emphasis on predicting "winners" and "losers" among commercially, ecologically and culturally important species[3,4]. Understanding how multiple stressors will alter resilience and sustainability of ecosystems is thus a priority for marine scientists working across molecular to ecosystem scales.

Species and ecosystems respond to multiple stressors via multivariate changes in abiotic conditions and biotic interactions across a range of spatial and temporal scales, yet this is under-represented within current research programmes. Analyses of ecological responses to climate change are frequently communicated in generalized terms such as 'poleward range shifts', with drivers represented as trends in long-term averages across large spatial scales[5,6]. It is increasingly clear, however, that decadal-scale increases in mean climate are not the proximate drivers of organismal survival. Instead, vulnerability through mortality or sub-lethal performance and consequently species distributions respond more directly to shorter-term variation in environmental conditions including extreme 'climatic' events and anomalies[7,8]. Consequently, predictions may have little relevance for individual species, nor be appropriate for ecosystem status assessments at local to regional scales. Eutrophication studies suffer from similar problems of scale, being predominantly focused on localized coastal areas and results scaled up to produce 'regional' generalized trends[9]. Such extrapolation can produce misleading or incorrect biological impacts forecasts due to a poor understanding of the biotic response mechanisms to changes in water chemistry in different locations. In stark contrast, due to inherent difficulties in studying impacts within natural systems, research into ocean acidification has focused on detailed physiological and organismal scale experiments conducted in small, controlled mesocosms or natural experimental areas, although there is a recognized need for larger scale approaches.

Small scale physiological studies provide yardsticks to gauge the sensitivity of organisms to changes in their environment, but their applicability to observable patterns in nature is difficult to assess due to the often single-species approach taken, and discipline-specific narrow focus adopted. Importantly, the stressors of greatest concern resulting from changing climatic conditions, temperature and ocean acidification frequently interact with one another and with other non-climatic stressors such as eutrophication, which subsequently alter sublethal responses within the same species[10,11]. To avoid potential misinterpretations we propose that expectations of how climate, OA and eutrophication are likely to affect ecologically important species should be based on ecologically-functional trait based metrics over appropriate spatial and temporal scales[12-14]. Such predictions should emphasize how multiple stressors interact to drive local-scale processes, and acknowledge the often overriding importance of biological responses and interactions in determining patterns of vulnerability over multiple spatio-temporal scales.

Rationale

The proposed INSHORE (International Network for the Study of How Organisms Respond to Environmental change) Working Group will employ a multi-disciplinary approach, integrating analyses of functional mechanisms and ecological processes with climatic and ocean chemistry data to provide realistic insights into the effects of global change on marine biological systems. Using an organism-to-ecosystem perspective we will develop a multiple stressor version of a dynamic bioclimate envelope model (DBEM) and methodological best practice guide for data collection and analysis to enhance our understanding of the most important and appropriate aspects of the responses of coastal marine species and ecosystems to global change.

We recognize that scientists cannot account for every possible combination of environmental conditions when forecasting ecological responses to global change. Rather, our central tenet is to determine what comprises an appropriate test of model skill and stationarity, meaning that models constructed from contemporary observations can effectively predict responses under future, often novel, environments[15]. To be effective, forecasts need to capture bio/eco-logically relevant stressor metrics[1,2,8,14,16,17], over appropriate spatio-temporal scales (10-100kms) applicable to the scientific research agenda and national and international policy drivers[12] (e.g. EU Marine Strategy Framework Directive, Water Framework Directive).

The Working and Associate Group members will review existing climate and ocean acidification models alongside published experimental research and methodologies for climate, ocean acidification and eutrophication experiments and studies for rocky intertidal systems. From this review and expert knowledge within the group a best practice guide to designing and carrying out experimental and observational studies to deliver fit-for-purpose data for use in multiple stressor modeling will be prepared and submitted for publication in PLOS One.

We will integrate detailed information on the mechanistic biology of species from experimental studies with molecular, physiological and ecological data[14,16,17,18], biogeographical time-series[8,19-21] and environmental datasets[22,23] within a macro-scale DEBM, sensu[24,25]. The DEBM will use these data to simultaneously estimate impacts of temperature, pH and nutrient levels on physiological performance, population dynamics, and dispersal to generate predictions of the impacts of multiple stressors on the biogeographic distributions of intertidal species. Model outputs will be created at a regional scale (100s km) within areas of the Atlantic and Pacific for which physiological, ecological, biogeographical and environmental data exist (e.g.[19,26]).

Rocky intertidal systems provide a highly tractable, data-rich system in which to develop and test such models. An important component of coastal habitats globally, they underpin both benthic and pelagic food webs, represent an important carbon pathway and support many species of both commercial and conservation value. The rocky intertidal also represents some of the most extreme and dynamic habitats in the marine realm. Organisms inhabiting this highly variable system are subject to high selection pressure arising from diurnal, seasonal and interannual fluctuations in environmental drivers and biological interactions[27] and are at high risk from multiple human-induced pressures, exhibiting some of the fastest responses to global change in any natural system[8,19].

The INSHORE Working and Associate Groups comprise researchers with international track records and ongoing research projects determining the impacts of climate change, OA and other human stressors on intertidal ecosystems. Expertise spans marine biodiversity time-series data collection and analysis (Mieszkowska, Russell, Lima), biogeography, macroecology and population ecology (Mieszkowska, Helmuth, Harley, Williams, McQuaid, Broitman, Fawzi, Chan, Christopholetti), physiological and behavioral experimentation (Russell, Sarà, Williams, Dong, McQuaid, Kroeker, Rilov) and modelling (Sarà, Helmuth, Williams, Mieszkowska), molecular transcriptomics (Dong, Williams), dynamic energy budget modeling (Sará, Helmuth, Williams), ecological climate impacts modeling (Broitman, Helmuth, Lima, Fawzi, Harley), climate and OA modelling (Broitman, Lima). Several members have previously collaborated and published together as evidenced by the cited research in this proposal.

A SCOR Working Group grant will provide a unique mechanism by which world-leading researchers with complementary cross-cutting, multi-disciplinary expertise can develop a novel, standardized multidisciplinary approach to research on multiple stressor impacts. This scope does not fall within the remit of national research council funding, given the variety of biological, spatial and temporal scales at which such questions need to be addressed. The wide geographical spread of expertise and datasets, and the global distribution of rocky intertidal systems far exceeds geographical boundaries defining existing regional or bi-national funding schemes (e.g. NSF, EU Horizons 2020).

The proposed topic of advancing multiple stressor impacts research via an integrated, international approach is timely given the major findings of the 2014 IPCC Report on Impacts, Adaptation and Vulnerability[28] that CO_2 emissions are driving unprecedented changes in global marine climate and ocean pH, multiple stressors 'impinge on resilience from many directions' and may be 'irreversible in terms of possible futures'. This knowledge gap with respect to marine ecosystems is also identified within the EU Marine Strategy Framework Directive[29]. Given these needs, this Working Group could be instrumental in leading a global, standardized approach to detecting, quantifying and predicting the impacts of multiple stressors on marine systems.

Terms of Reference

INSHORE will pursue the following terms of reference:

1. Disseminate the Working Group activities and outputs via: development of a website with associated blog and Twitter account; hosting targeted sessions on multiple-stressor impacts research at major international meetings to increase awareness and engage scientists from multiple countries with the need for a standardized, multi-disciplinary approach to address this complex problem.
2. Create a database of relevant biogeographical, ecological, biological and environmental datasets held by, and accessible to the group.
3. Review existing climate models and ecological, biological and physiological experimental research into climate change, ocean acidification and eutrophication to develop a best practice for integrated multiple stressor research protocols. These best-practice approaches will consolidate the international research effort into marine climate change and provide standard protocols by which scientists new to this research field can produce comparable, robust data across research groups and nations.
4. Produce a best practice methodology and a case study output for the region of each Working Group member using the multiple stressor model.
5. Develop and test a next generation multiple stressor impacts model using existing time-series, experimental and environmental datasets collated in ToR 2.

Working plan

To achieve its goal INSHORE will:

(1) integrate an international Working Group with expertise in physical, ecological, physiological and molecular sciences which will have the goal of developing a novel multiple stressor profiling model. This model will assess recent change and forecast future impacts of short-term weather and decadal-scale climate on biodiversity, functioning and resilience of rocky intertidal ecosystems.

(2) to initiate this model, the group will utilize their unique wealth of scientific and monitoring datasets as well as those collected by the wider global marine climate research community including existing data repositories (e.g. ICES, PICES, OBIS, EMODnet, Redmap) and time-series such as the UK MarClim dataset (led by CoChair Mieszkowska) and Pacific USA dataset (Broitman) to create a dataset of biogeographic distributions, species traits (e.g. thermotolerance), lifecycle dynamics and population abundances for rocky intertidal ecological-engineer species. These data will be entered into a purpose-built database and used to derive best practice methodologies and to develop and test the DBEM.

(3) Based on the outcomes from (2) the experts in climate impacts modeling from the Working Group and Associate Members will lead a review of their own and other existing global change impacts models with input on novel methodologies and parameters necessary to develop next generation multiple stressor models provided by the Working Group and Associate experts.

(5) Assessment of species-specific physiological performances and tolerances, changes to trophic interactions, and macroecological data on distributional range shifts and abundances will be integrated with the climate models in a context of IPCC AR-5 scenarios (2014) to develop a Dynamic Biostressor Envelope Model that will provide quantitative assessments of the future vulnerability of organisms and ecosystems to climate change.

(6) Finally, the model outputs will be designed at spatio-temporal scales relevant to policy and management drivers including OSPAR Regions, EU Regional Seas and Marine Protected Areas (e.g. the Australian Representative Network of MPAs, UK Marine Conservation Zone and Special Areas of Conservation Networks, EU MPA Network) and disseminated via the INSHORE website and direct communication from Working Group members to policymakers via existing science-policy groups such as the UK Healthy and Biologically Diverse Seas Evidence Group, Marine Climate Change Impacts Partnership, Australian National Climate Change Research Facility).

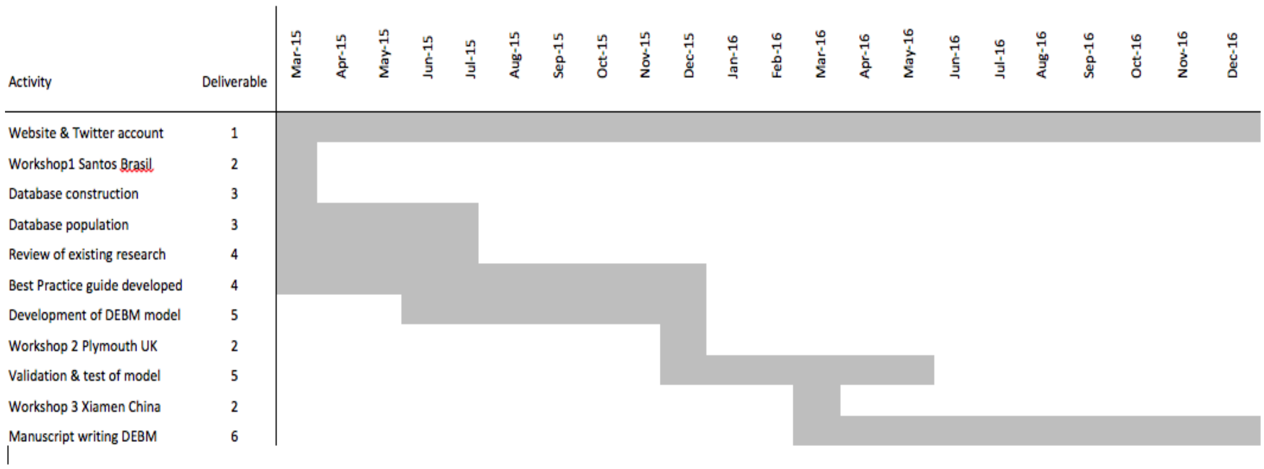
Timeline

The first INSHORE working group meeting will be a three day workshop and themed session held at the 'Third International Symposium on Effects of Climate Change on the World's Oceans', 23-27 March 2015 in Santos, Brazil. This meeting is coordinated by ICES and sister affiliations the North Pacific Marine Science Organization (PICES) and the Intergovernmental Oceanographic Commission of UNESCO (IOC-UNESCO). The driver is a recognized symbiosis between the oceans and society, underpinned by the role of science, and a need for the assessment of the consequences of climate change on the world's waters, ecosystems and living resources. The associated SCOR workshop will be organized by Co-Chair Mieszkowska and INSHORE Associate Member Christofoletti, from the conference host institute Universidade Federal de São Paulo, who will cover venue costs as an 'in kind' contribution. The workshop and themed session will be open to participation by students from Instituto do Mar and other registered participants of the conference. Working Group members will present relevant research at the symposium and participate in the workshop.

This meeting will involve presentations of working group members' research activities and launch of a website (Term of Reference 1, Deliverables 1,2), the construction and population of a meta-database of relevant biogeographical, ecological, biological and environmental datasets held by, or accessible to the group (ToR 2, Deliverable 3), a review of existing climate models will be carried out (ToR 3, Deliverable 4) and a best practice guide for multiple stressor impacts research in coastal marine systems drafted (ToR 4, Deliverable 4). Presentations on the state of climate impacts modeling and availability of datasets for climate, OA and eutrophication at ocean basin, national and regional scales will be given by Broitman, Helmuth, Lima, Kroeker, Harley, Fawzi and Mieszkowska who are world-leaders in this field. Ecological responses to multiple stressors will be presented by Williams, Harley, McQuaid, Helmuth, Chan and Christofolettii. Williams, McQuaid, Dong, Sarà, Rilov and Mieszkowska will present work on molecular and physiological single and multiple stressor research. Discussions between the group members will include datasets to be incorporated into the new multiple stressor model and an agreed time-line for remote participation and delivery of data to the modelers.

A second workshop will be held at the end of 2015 at the Marine Biological Association, Plymouth, UK. Co-Chair Mieszkowska will host the four day workshop, with venue costs covered as an 'in-kind' contribution. The developing DEBM model will be showcased at this workshop and the working group will test and validate the model using the metadatabase collated at the first workshop in Brasil (ToR 5, Deliverable 5). Between workshops two and three the review manuscript of the status of the marine multiple stressor research field will be written by the Working Group using cloud file sharing and virtual group working methods successfully employed by members for previous publications.

A final workshop will be held in early 2016 at Xiamen University, China, hosted by Working Group member Dong. Here the working group will test the final version of the model with datasets held by the Working Group and perform model runs targeted at regional scales relevant to management of adaptation strategies, harvest of commercially important species, and zonation and planning of Marine Protected Area networks. The working group will write a manuscript on the DEBM model using this case study for submission by the end of 2016 (Deliverable 6).



Deliverables

The WG will provide a mechanistic approach to understanding how coastal marine species and ecosystems will respond to climate change, ocean acidification and eutrophication to challenge the paradigm of predictions based on existing time-series and physiological data from the ICES community and new, high resolution (10-100 kilometers) environmental data.

Specific outputs are to:

1) Launch a website and Twitter account providing information on the project activities, model outputs and links to related ICES activities.
2) Present Working Group expertise in multiple stressor research and promote the ongoing activities of the Working Group at international scientific meetings.
3) Create a database of biological and environmental datasets for use in developing and the best practice guide (4) and testing the multiple stressor model (5).
4) Publish a review of existing climate models alongside a best practice guide of the multidisciplinary, integrated methodological approach to next generation multiple stressor profiling modeling in the open access international journal PLOS One.
5) Develop a novel DEBM multiple stressor profiling model and make the code available to the international marine research community.
6) Publish model codes and outputs in international journals (e.g. Ecological Modelling, Global Change Biology) highlighting the roles of climate, ocean acidification and eutrophication in shaping and changing intertidal ecosystems.

Capacity Building

The INSHORE Working Group membership encompasses researchers from developing nations (Chile, South Africa, China, Iraq) and associate members from Brasil, Israel and Taiwan. INSHORE comprises ten Working Group members and five Associate members spanning early to mid career international researchers (Mieszkowska, Broitman, Harley, Russell, Sarà, Dong, Kroeker, Lima), and international experts in global change biology running research institutes and university departments (Helmuth, Williams, McQuaid, Fawzi).

The membership of leading scientists in global change impacts spans all major continents to ensure an international scope for the exchange of knowledge, data and expertise. The range of expertise from molecular genetics through physiology, biology, ecology to climate modeling will ensure exchange of knowledge and skills between participants and nations. SCOR Working Group funding would allow the individual members to foster long-term collaborative working relationships and facilitate continued exchange of skills and expertise across developed and developing nations that would not be possible under other existing funding opportunities (e.g. research council or regional networking grants).

The group will present their contributions to an integrated multiple stressor research perspective at the Third International Symposium on Effects of Climate Change on the World's Oceans in Brasil, and host workshops to develop the integrated methodology and associated multiple stressor profiling model in Brasil, China and the UK. The Brasil conference will be attended by PICES and ICES member nations researchers ensuring an international scientific audience, as well as the international science-policy community via the Intergovernmental Oceanographic Commission of UNESCO (IOC-UNESCO). This global science-policy meeting is a high profile venue for the dissemination of the Working Group’s activities and best practice integrated research programme.

Students from host and local institutes will be invited to interact with the global Working Group at these events, and Working Group members will give presentations on this project at host universities and associated research laboratories. These dissemination activities will promote the INSHORE project to the benthic research communities and early career scientists and students associated with the Working Group members and workshop host institutes in South and North America, Europe, Africa, Asia and Australasia.

An INSHORE project website will be set up with an associated blog and Twitter account to provide continuous dissemination of project activities and outputs, including the DEBM model methodology and code and the best practice guide that will be promoted as an integrated standard approach within the global change research community. The website will be linked to the SCOR website and all Working Group and Associate Member laboratory websites. This will provide a lasting, open access record of achievements and activities, and facilitate exchange and sharing of experimental approaches developed across member countries.

Working Group composition
Full Members

Name	Gender	Place of work	Expertise relevant to proposal
1 Nova Mieszkowska	Female	Research Fellow, Marine Biological Association of the UK	CoChair. PI, MarClim; most spatio-temporally extensive intertidal species time-series globally. Macroecological responses to multiple stressors. Mesocosm and field experimental physiology; responses to climate, OA, nutrients. PI national research grants on climate change and OA impacts on marine biodiversity.
2 Gray Williams	Male	Director, The SWIRE Institute of Marine Science, University of Hong Kong	CoChair. 20+year experience in tropical intertidal ecology: field and laboratory approaches to physiological responses and impacts on local and regional community dynamics. Large-scale latitudinal projects in Japan, China, Vietnam, Thailand, Malaysia, Singapore.
3 Brian Helmuth	Male	Director, Sustainability Science and Policy Initiative. Professor, College of Science, Northeastern University, USA	Ecological forecasting, physiological mechanistic responses to climate, thermal engineering technology, mathematical modeling.
4 Bernardo Broitman	Male	Director, Centro de Estudios Avanzados en Zonas Aridas, Santiago, Chile Associate Professor, Facultad de Ciencias del Mar, Universidad Catolica del Norte,Chile.	Community ecology, responses of coastal organisms to climate. Environmental modelling, coastal oceanography. PI most extensive coastal observation network on the Southeast Pacific. Deputy Director, MUSELS multiple stressor research centre.
5 Christopher McQuaid	Male	Chair of Zoology and SARCHI Research Chair in Marine Biology, Rhodes University, South Africa	Substantial track record in ecology of benthic ecosystems, species interactions, invasive species, climate change. Importance of multiple stressors through multiple spatial scale experiments.
6 Chris Harley	Male	Associate Professor, Department of Zoology, University of British Columbia, Canada	Impacts of climate and OA on coastal ecology. Physiological responses of intertidal invertebrates and macroalgae.
7Yunwei Dong	Male	Professor, State Key Laboratory of Environmental Science, Xiamen University, China	Physiological and molecular (transcriptomics, proteomics) responses of intertidal invertebrates to multiple stressors.
8 Nadia Al-Mudaffar Fawzi	Female	Head of Department, Biological and at Marine Science Centre, University of Basra, Iraq	Impacts of anthropogenic stressors on coastal ecosystems. Eutrophication & water quality research programme.
9 Bayden Russell	Male	Southern Seas Laboratory, University of Adelaide, Australia	Experimental assessment of physiological changes and resultant ecosystem functioning due to eutrophication, CO_2, temperature through primary productivity and trophic interactions.
10 Gianluca Sará	Male	Associate Professor, Department of Earth and Marine Science, University of Palermo, Italy	Experimental estimation of functional traits under multiple stressors to feed Dynamic Energy Budget models assessing life-history traits of bentho-demersal organisms.

Associate Members

Name	Gender	Place of work	Expertise relevant to proposal
1 Fernando Lima	Male	Centro de Investigação em Biodiversidade e Recursos Genéticos, Portugal	Biogeography of intertidal organisms, climatic reconstruction and analysis, modelling.
2 Kristy Kroeker	Female		OA impacts on marine invertebrates.
3 Ronaldo Christofolettii	Male	Instituto do Mar, Universidade Federal de São Paulo, Brasil	Trophic interactions within intertidal ecosystems.
4 Benny Chan	Male	Principal Scientist & Associate Professor, Coastal Research Laboratory, Academia Sinica, Taiwan	Intertidal, supply-side and larval ecology, biogeography of tropical intertidal invertebrates.
5 Gil Rilov	Male	Senior Scientist, National Institute of Oceanography, Israel	Community biodiversity, biogeography, benthic-pelagic coupling. Multiple stressor mesocosm and long-term field programme.

Working Group Contributions

Mieszkowska. International track record spanning biogeographical to molecular impacts of global change on intertidal species and ecosystems. PI and primary data collector of world-leading UK MarClim Project and New Zealand, Australian and Icelandic sister projects with associated extensive experimental mesocosm and field datasets for physiological impacts of multiple stressors.

Williams. Established the first trans-Chinese field time-series of biophysical and environmental sensor network within rocky intertidal habitats, leads internationally renowned SWIRE Institute research programme into multiple stressor impacts on intertidal systems.

Helmuth. World leader in thermal engineering, energetics and bioclimate research using intertidal ecosystems as a testbed for NASA and NSF funded climate modeling projects. Leads biophysical experimetnal latitudinal research projects along Atlantic coastline of USA.

Broitman. Internationally acclaimed bioclimate modeler, PI of most extensive Pacific intertidal time-series dataset, PI of Chilean research programme into multiple stressor impacts on marine systems.

McQuaid. South African National Research Foundation ‘A rated’ researcher with a global profile in environmental impacts on intertidal systems, McQuaid has held posts including Director of the Southern Ocean Group (SOG) at Rhodes University for 20 years, South African Research Chair (SARChI) in Marine Ecosystem Research at Rhodes University. Holds extensive datasets for South African intertidal.

Harley. Leading expert in field experimental research into impacts of climate change and ocean acidification on species physiology and ecology, community structure and functioning.

Dong. Driving cutting-edge physiological and molecular techniques for application to mechanistic research into responses of marine intertidal species to environmental stress. Leading the Chinese research drive into climate change impacts.

Fawzi. Leading authority in Iraq for water quality and impacts on coastal ecosystems. Heads research efforts into eutrophication and pollution research in the Persian Gulf system.

Russell. Expert in experimental testing of multiple stressor impacts on macroalgae and trophic interactions via development of state-of-the-art mesocosm systems. High impact publication record for climate change and ocean acidification impacts on macroalgae, with associated field and experimental datasets for Australia.

Sará. Developed dynamic energy budget models that have been adopted as the international standard for coastal marine invertebrate species. IPCC AR5 national reviewer and research co-ordinator for Italian-Asian binational research networks.

Relationship to other international programmes and SCOR Working Groups

INSHORE will link to existing international working groups and research networks via the proposed Working Group and Associate members. This will ensure wider knowledge exchange, continued dialogue and ensure complementarity without overlap between the various networks. These include:

- GRIEN Global Rocky Intertidal Ecology Network that involves field monitoring of intertidal biodiversity and environmental parameters, led by Dr Gil Rilov and involving Working Group members Mieszkowska, Williams, Helmuth, Sará, Harley and McQuaid.
- Ocean Acidification Network led by Dr Kristy Kroeker and involving Working Group members Russell and Harley.
- Millennium Nucleus Center for the study of multiple-drivers on marine socio-ecological systems - MUSELS, investigating the effects of environmental and socioeconomic drivers on the shellfish farming industry both in northern and southern Chile, PI Working Group member Broitman.

No current SCOR Working Groups are investigating global change multiple stressor impacts, but INSHORE will continue to monitor the activities of all Working Groups including WG137 that is collating large datasets on plankton distributions via an international database similar to the one planned for benthic species through INSHORE.

Key References

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Appendix

Five key publications per Working Group Member (author and co-authors who are also WG members highlighted in bold):

Mieszkowska

1. **Mieszkowska N.**, Burrows M., Pannacciulli, F. & Hawkins, S.J. 2014. Multidecadal signals within co-occuring intertidal barnacles *Semibalanus balanoides* and *Chthamalus* spp. linked to the Atlantic Multidecadal Oscillation. 10.1016/j.jmarsys.201211008.
2. **Mieszkowska, N**., Sugden, H. Firth, L. & Hawkins, S.J. 2014. The role of sustained observations in tracking impacts of environmental change on marine biodiversity and ecosystems. Philosophical Transactions of the Royal Society A, in press.
3. **Mieszkowska, N**., Milligan, G., Burrows, M.T., Freckleton, R. and Spencer, M. 2013. Dynamic species distribution models from categorical survey data. Journal of Animal Ecology 82(6) 1215-1226.
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Williams

1. Marshall, D. J., **Dong, Y. W., McQuaid, C.D.,** & **Williams, G.A. (**2011). Thermal adaptation in the intertidal snail Echinolittorina malaccana contradicts current theory by revealing the crucial roles of resting metabolism. *The Journal of experimental biology*, *214*(21), 3649-3657.
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Helmuth

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McQuaid

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Harley

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Dong

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Proposal for a SCOR working group on
Patterns in global plankton biogeography

Acronym: MARBIOG

Abstract

Marine planktic ecosystems respond to changes in environmental conditions such as global warming and ocean acidification, but they also drive global biogeochemical cycles themselves. Thus, a major reorganization in plankton biogeography due to climate change will feed back onto climate and global biogeochemical cycling by modulating ocean CO_2 storage and emissions of climatically important trace gases. Recently, the MARine Ecosystem DATa (MAREDAT) initiative brought together over 500’000 abundance and biomass measurements. For the first time, it is now possible to investigate plankton biogeography at the global scale, and within the context of a diverse set of applications from marine ecosystem model validation to applications in theoretical ecology. However, the MAREDAT data set is inhomogeneous, and has strong biases due to inconsistent sampling and data recording strategies. In order to fully understand plankton biogeography, a pairing with physiological trait data is essential. Here, we propose a SCOR working group on the analysis of plankton biogeography. The SCOR group would develop new protocols for the reporting and collection of global-scale planktic ecosystem data relevant for ocean biogeochemical cycles and macroecology, and would extend the current MAREDAT collection. We propose to include geo-referenced abundance/biomass and plankton physiological traits as well as biological rates in the next version of MAREDAT, and to analyse global patterns of plankton and trait biogeography across multiple trophic levels. We will synthesize data on both zooplankton and phytoplankton, develop tools to extrapolate scarce biological data to global scales, and compare global patterns of trait and plankton biogeography and diversity.

1. Scientific Background and Rationale

Anthropogenic climate change has been shown to impact marine planktic ecosystems in several crucial ways: On a global scale, the ocean is simultaneously undergoing warming, deoxygenation and acidification (Doney, 2010); that is, the ocean is “warming up, losing breath, and turning sour” (Gruber, 2011). Increased stratification in subtropical and temperate latitudes may limit nutrient availability and decrease primary productivity over this century (Steinacher et al. 2010). These changes may already be underway: the oligotrophic regions of the oceans appear to be expanding (Polovina et al. 2008), Pacific species have been shown to migrate into the Atlantic (Reid et al. 2001), zooplankton species shifts have been recorded in the North Atlantic (Beaugrand et al. 2004, 2008), and regime shifts have occurred in the Black and Caspian seas (Oguz & Gilbert, 2007). These and many more studies show that anthropogenic impacts affect ecosystems across multiple trophic levels and in many different ways (Doney et al. 2012).

Marine planktic ecosystems play an important role in the global biogeochemical cycling of key elements such as carbon, nitrogen and sulfur. Marine plankton form the base of the food web, and are of crucial importance for everything from the marine biological pump and ocean CO_2 storage to global fisheries and food security. Specific plankton groups produce nitrogen, sulfur and organohalide trace gases that can affect climate and atmospheric chemistry. Marine biodiversity forms a resource that is exploited in many industrial ways from the use of genes that code for low-temperature enzymes in detergents, to food supplies and animal food stocks. However, many marine ecosystem services related to global biogeochemical cycling, food provision and genetic diversity are still poorly quantified (Worm et al. 2006), since few aspects of marine ecosystem structure and composition are routinely monitored on the global scale. Thus, changes in marine ecosystem structure and functioning may crucially impact global climate and the livelihood of millions of people relying on marine resources. The FAO estimates that about one billion people worldwide rely on fish as their primary source of animal protein (FAO, 2000).

Recent advances in remote sensing now allow the estimation of different plankton functional types (PFTs) and size structure from space using water-leaving reflectance (Alvain et al. 2005, Hirata et al. 2008, 2011) or backscattering (Kostadinov et al. 2009, 2010), with prospects for long-term monitoring. However, most remote sensing algorithms have been validated using only a few hundred data points in limited ocean regions (e.g. Hirata et al. 2011, Alvain et al. 2012). Extensive sets of validation data are essential in order to use the high-resolution products to monitor patterns of change on the synoptic global scale. In order to quantify potential future change, ecosystem model simulations are required (Bopp et al. 2001, Hashioka et al. 2009, Steinacher et al. 2010). Marine ecosystem models are becoming increasingly complex (Follows et al. 2007), and the availability of trait data for their parameterization, and biomass data for their evaluation, is an important determinant in the rate of progress (Le Quéré et al. 2005, Litchman et al. 2006).

Recent years have seen an exponential increase in the availability of plankton trait data. Published phytoplankton trait data comprise maximum growth rates and nutrient, light and temperature responses (Klausmeier et al. 2004; Litchman et al. 2007, Litchman and Klausmeier 2008; Edwards et al. 2012; Thomas et al. 2012). Zooplankton trait data on size distribution, feeding strategies and behavioral patterns are also abundantly available (Forster et al. 2011, Kiørboe, 2008, Kiørboe 2011). Yet, an understanding of marine ecosystem structure and functioning based on first principles of ecology remains elusive, as high observational coverage remains limited to a few regions. In their recent review, Barton et al. (2013) suggest that an initiative to collect trait data in a concerted manner similar to MAREDAT is essential for further progress on the understanding of marine planktic ecosystem structure and functioning.

The MAREDAT2012 atlas of PFT abundance and biomass, compiled by members of this group, published publically available databases and peer-reviewed documentation. The analysis of the datasets is under way (Brun et al. in prep.; Vogt et al. in prep.; O'Brien et al., in prep.), and initial results reveal exciting insights into plankton biodiversity and biogeography. Yet, methodological and sampling biases are present, which need to be addressed in order to understand plankton community structure and its vulnerability to global change: (1) inconsistency in the reporting of species information, (2) bias due to inconsistent sampling methods, (3) seasonal and regional bias, and (4) does not include all existing data. While these issues were unavoidable in a first round of data collection, some can be addressed in a second round, and global standards can be set in a joint international effort.

In terrestrial ecosystems, trait and abundance measures have been combined into multiple indices of, for example, functional diversity, which is shown to relate to the magnitude of ecosystem services (e.g. Randerson et al. 2009; Clark et al. 2012). In order to quantify marine ecosystem services, a similar effort is necessary to understand, model and predict present and future changes in marine planktic ecosystems, and their consequences for ecosystem service provision. The systematic data collection we propose opens the door for a variety of different applications:
1) predict spatio-temporal patterns in species characteristics (Edwards et al. 2012, Thomas et al. 2012),
2) elucidate biodiversity patterns (O'Brien et al., in prep., Worm et al. 2006, Irigoien et al. 2004, Rutherford et al. 1999),
3) study the flow of matter across different trophic levels (Buitenhuis et al. 2013b),
4) study ecological niches of plankton species (Brun et al., in prep., Irwin et al. 2012),
5) investigate species and biome shifts in marine planktic ecosystems (e.g. Beaugrand, 2004, Beaugrand et al. 2008, Alvain et al. 2013),
6) assess global patterns of elemental ratios that are crucial for global biogeochemical cycling (Martiny et al. 2013),
7) determine the drivers of plankton biogeography (Dutkiewicz et al. 2012, Luo et al., 2014),
8) quantify ecosystem services related to global biogeochemical cycling, such as primary production (Buitenhuis et al. 2013b) nitrogen fixation (Luo et al. 2014), DMS production (Schoemann et al. 2005), and opal production and export (Sarmiento and Gruber, 2006),
9) calibrate remote sensing algorithms of phytoplankton groups (Alvain et al. 2012, 2013, Hirata et al. 2011).

1.3 Timeliness and relevance of the activity

The proposed activity is timely, as global data sets have only recently become available, and standards for their formats, archiving and quality control have not yet been set. Defining standards and joint interpretation will provide added value and will speed up research on the impact of climate change on marine ecosystems.

1.4 Relevance for SCOR sponsorship

This proposal addresses a topic at the forefront of current marine ecosystem research, focusing on global patterns of marine biogeography and potential changes in marine ecosystem structure and functioning, and will solve essential methodological and ecological questions that would otherwise remain unanswered were it not for the synergy between MAREDAT, international data archives such as ICSU's World Data System, GBIF, EMODnet and others, and the physiological/ecological trait communities that a SCOR working group provides on an international level. It would allow the participants to address ecological questions across multiple trophic levels by specifically tailoring the new plankton atlas to the scientific questions it aims to address. The working group would allow the combination of global scale information on ecosystem function and trait biogeography with information on community structure and plankton distribution, for example to address the role of biodiversity and functional diversity for ecosystem functioning and ecosystem service provision.

2. Terms of Reference

The proposed working group would

(1) summarize and assess the current availability of experimental and field measurements of plankton abundance, biomass, pigments and traits
(2) collaborate with data archives such as PANGAEA, BCO-DMO, and COPEPOD, and with SeaDataNet, the ICSU World Data System, the IMBER data management group, EMODnet, GBIF and others in order to develop and publish a comprehensive *Guide of standard protocols and best practices for the compilation of plankton data*, including specifications about data citation, geolocation, collection methods, standard parameter vocabularies & units, and quality control
(3) publish a new open access atlas of marine plankton abundance and biomass data (MAREDAT2017) and a collection of geo-referenced and in situ life history and physiological trait data across multiple trophic levels in marine ecosystems.
(4) develop and disseminate new methods to interpolate scarce biological data to scales relevant to address important concepts of theoretical ecology and to quantify important ecosystem services provided by marine ecosystems, using statistical tools from terrestrial ecosystem research and important concepts of theoretical ecology, and the quantification of important ecosystem services.
(5) generate a knowledge base of taxon-specific and phylogenetic-specific traits for the full size spectrum of plankton, i.e. from viruses to large planktonic metazoans and inform the observational community of our data needs and current gaps in our understanding of marine ecosystem structure and functioning.
(6) joint analyses of global patterns in trait and plankton biogeography and diversity and their role for marine ecosystem functioning across multiple trophic levels.

3. Working Plan

The workflow is broken down into 3 work packages.

Work package 1. Synthesis of plankton biomass data and plankton biogeography: WP1 will produce an update of the MAREDAT2012 first global atlas of marine plankton functional type abundance and biomass data in 2017. MAREDAT2017 will contain at least 14 contributions: updates of the 12 databases in MAREDAT2012 for diatoms (Leblanc et al. 2012), coccolithophores (O'Brien et al. 2013), nitrogen fixers (Luo et al. 2012), *Phaeocystis* (Vogt et al. 2012), picophytoplankton (Buitenhuis et al. 2012a), bacteria (Buitenhuis et al. 2012b), micro- (Buitenhuis et al. 2010, 2013a), meso- (Moriarty and O'Brien, 2012) macrozooplankton (Moriarty et al. 2013), pteropods (Bednarsek et al. 2012) and planktic foraminifers (Schiebel and Movellan 2012), as well as HPLC pigments (Peloquin et al. 2013). In addition, an update of the World Ocean Atlas Chlorophyll *a* database (Conkright et al. 2002) will be included, as well as a new database on autotrophic/mixotrophic dinoflagellates. We will also solicit contributions on gelatinous plankton, virioplankton and planktic species in palaeoceanographic sediment records.

Work package 2. Synthesis of plankton life history traits: WP2 will generate a knowledge base of taxon-specific traits for the full size spectrum of plankton (MARETRAIT), which will be included in the taxonomic register WoRMS. WP2 will produce comparisons of phytoplankton and zooplankton traits across size classes, and of trait biogeography across multiple trophic levels. The zooplankton traits will include grazing rate and respiration rate as a function of temperature, assimilation and gross growth efficiency, and DOM exudation (Buitenhuis et al. 2006, 2010, Kiørboe and Hirst 2014). The phytoplankton traits will include intra- and inter-PFT changes in growth rate with cell size (Le Quere et al. in prep.), temperature dependence of growth rate (Buitenhuis et al. 2013b; Thomas et al. 2012) and nutrient uptake traits (Klausmeier et al. 2004; Litchman et al. 2007, Edwards et al. 2012). This WP will also address the issue of compatibility between geo-referenced and laboratory trait data, and develop recommendations for the collection, reporting and use of these different data types.

Work package 3 Understanding marine ecosystem structure and functioning: WP3 will combine trait and biomass data to further our understanding of marine ecosystem function. It will develop and test statistical techniques for the extrapolation of scarce biological data to larger scales, using methods common in species distribution modeling. It will build on the MAREDAT2017 and MARETRAIT datasets, and the EURO-BASIN special issue which includes key links between planktic systems and ecosystem services. WP3 will quantify fluxes between the different trophic levels, and assess links between different forms of diversity and the magnitude of ecosystem services related to biogeochemical cycling and food-web dynamics. WP3 will also identify gaps in our understanding of marine ecosystems and associated data needs, and publish a joint paper on this issue.

Pre-meeting: The members of the proposed SCOR working group will attend the IMBER Open Science Conference in Bergen in June 2014, but it will not rely on SCOR funding. A pre-meeting will take place after a common session between the trait and biomass community on: "Data synthesis and modeling of marine planktic ecosystems with plankton functional types and trait-based models". This session invites discussion between members of trait ecology and plankton biogeography on how to combine abundance and biomass data with trait and pigment data, and how to link them for a better quantification of ecosystem services.

Kick-Off Meeting: In order to provide international visibility and assure high attendance, the kick-off meeting would coincide with a relevant international conference, probably the ASLO Aquatic Sciences meeting in 2015 in Granada, Spain. We will organize a 2-day workshop after the meeting where data collection strategies will be coordinated.

Further meeting: A second business meeting would be organized in 2016 during the Ocean Sciences conference in New Orleans. During this meeting, the progress of data collection and publication would be reviewed, and the guidelines for data standards re-evaluated.

Workshop: In the beginning of 2017, the proposed SCOR working group would host a workshop at the University of East Anglia. WP1 will discuss ongoing and new scientific collaborations to exploit the MAREDAT2017 databases (e.g. ecological niche determination, gap filling algorithms, bottom-up / top-down interactions). WP2 will finalise the zooplankton trait intercomparison and discuss the phytoplankton trait intercomparison. Both groups together will discuss mathematical tools to constrain PFT traits using biogeochemical models evaluated against the MAREDAT2017 databases. Furthermore, the group will coordinate the analysis of the collected data, i.e. identify lead authors for the planned set of synthesis papers. During the workshop, the group would generate an outline for the community white paper on our current understanding of marine ecosystem structure and functioning.

Final meeting: In 2018, members of this SCOR working group would meet either at the Ocean Sciences 2018 or at the ASLO meeting, and coordinate further joint analysis of the data collected.

Timeline of Milestones

Year 1 (2015):
A) Synthesis of protocols specific for each data type, method and plankton group (WP1&2).
B) Identification of ecological, physiological and morphological traits with sufficient data coverage, in space and time, to be included in MARETRAIT2017 (WP2).
C) Development and dissemination of guidelines for quality control (WP1&2).
D) Data call for MAREDAT2017 (WP1).

Year 2 (2016):
A) Data collection for the different plankton groups to be included in MAREDAT2017 (WP1).
B) Submission of individual MAREDAT2017 datasets and papers. (WP1).
C) Inclusion of taxon-specific traits in the taxonomic register WoRMS (WP2).

Year 3 (2017):
A) Publication of a standard protocols and software (WP1&2)
B) Workshop at UEA (WP1&2&3)
C) Papers analyzing phyto- and zooplankton trait biogeography across different PFTs (WP2)
D) Open access publication of final MAREDAT2017 papers and databases (WP1).

Year 4 (2018):
A) Submission of methods paper to interpolate scarce and highly variable biological data sets to larger scales (WP3).
B) Submission of a paper analyzing and comparing MAREDAT2017 biomass data across different taxonomic groups and trophic levels (WP1&3).
C) Submission of a paper analyzing links between phyto- and zooplankton biogeography and their respective patterns in trait distribution across different PFTs (WP3)

4. Deliverables

The main final products of the SCOR working group are the updated MAREDAT2017 atlas of global plankton biogeography by the end of 2016, consisting of a set of at least 14 papers on plankton abundance, biomass and pigment data; and a new MARETRAIT2017 atlas, with at least two papers on geo-referenced/laboratory trait data for zooplankton and phytoplankton and three synthesis papers that analyse the MAREDAT and MARETRAIT databases across all groups and links between plankton biogeography and global patterns in trait distribution. A guide will be published with data format and quality control recommendations, including taxonomic specification, and standard units for abundance, biomass, pigment and trait data to make them suitable for a wide set of applications in biological oceanography and marine ecosystem modeling. Common software will be created and published on the MAREDAT website (www.maredat.info) that handles (1) the quality control procedure, (2) the generation of gridded products, and (3) routines for the interpolation of data to larger scales using novel techniques (e.g., Lana et al. 2011; Landschützer et al., 2013). A white paper will be written by the end of year 3 that identifies gaps in our current understanding of marine ecosystem structure and functioning, and details the data needed to address these. A joint interpretation of the data and recommendations will also be highlighted in a high-profile publication written by the group in year 4.

5. Capacity building

From a socioeconomic perspective, many issues in current marine ecosystem research, such as the quantification of potential impacts of global change on marine ecosystem service provision is highly important for developing countries and economies in transition. The results of the proposed activity will inform policy makers and the public on potential hotspots of ecological change, and on locations with a high degree of diversity. The proposed SCOR working group would bring together the MAREDAT community with other marine ecologists, data archives, marine ecosystem modelers (e.g. MAREMIP initiative), and members of the remote sensing community. These communities have a common goal – the understanding of present and future marine ecosystem structure and functioning – but are currently not linked through an international working group. The SCOR working group would thus facilitate the important exchange of ecosystem data between different ecosystem researchers working toward a common goal. For example, the remote sensing community may require data for the evaluation of their algorithms, while marine ecosystem modelers will need physiological rates/trait data to implement further complexity into their models. A SCOR working group would also lead to the identification of data requirements and needs by these different communities, and how MAREDAT could accommodate a maximal set of such needs through sensible and simple data standards. Bringing these diverse communities together around a table would also increase the international visibility of marine ecosystem research, and will lead to future collaboration, ideas and findings. The SCOR working group would also increase efficiency in the expansion and establishment of global plankton data sets. The MAREDAT community already has experience with the generation of a global plankton atlas, and this know-how can be exploited by the trait community to collect and archive data more effectively. In addition, close contacts will be established with members of the terrestrial ecosystem community through the use of statistical tools and concepts that are common in terrestrial ecosystem research. Building necessary capacities in developing countries can be fostered by providing access to open-source data, best practice manuals and standard protocols that will augment access by members from countries with limited financial and infrastructural means to generate their own data. Additional funding would be requested from SCOR's travel grant program to finance the attendance of at least one additional young scientist from a developing country to attend international meetings, whenever the proposed SCOR group members meet. Thus, young scientists would be trained in essential networking and technical skills while being introduced to leading international members in the field.

6. Working Group Composition

Full members, chairs in bold

Name		Place of work	Expertise
Meike Vogt	F	ETH Zürich, Switzerland	Phytoplankton ecological niches and biogeochemistry, global plankton biogeography
Erik Buitenhuis	M	University of East Anglia, UK	Plankton ecology, global biogeochemical modelling, macroecology
Simon Claus	M	Flanders Marine Institute	Biodiversity patterns. Contact with EMODnet and WoRMS
Forough Fendereski	F	Gorgan University, Iran	Plankton biogeography and marine biomes
Takafumi Hirata	M	Hokkaido University, Japan	Detection of plankton functional groups from space
Xabier Irigoien	M	King Abdullah University of Science and Technology, Saudi-Arabia	Marine ecology, biodiversity
Thomas Kiørboe	M	DTU-Aqua, Denmark	Zooplankton ecology and traits
Elena Litchman	F	Michigan State University, USA	Phytoplankton ecology and traits
Yawei Luo	M	Xiamen University, China	Nitrogen cycling, traits of nitrogen fixers
Maria Deng Palomares	F	World Fish Centre, Philippines and University of British Columbia, Canada	Fish population dynamics

Associate members

Andrew Barton	M	Duke University, USA	Lower trophic level trait ecology, ecological modelling
Karine Leblanc	F	MIO CNRS, France	Diatom biology and silicon cycling
Stephane Pesant	M	Bremen University, Germany	Biological data collection, integration and publishing
Ralf Schiebel	M	University of Angers, France	foraminifera and palaeoceanography

7. Working Group Contributions

7.1 Full Members

1. **Meike Vogt**: Co-coordinator of MAREDAT2012 & 17. Collection of standardized plankton data for use in biological oceanography and ecosystem modeling. Standard protocols and data collection for use in model validation and marine ecology. Species distribution modelling and phytoplankton macroecology. Member of MAREMIP SSC.

2. **Erik Buitenhuis**: Co-coordinator of MAREDAT2012 & 17. Marine ecologist. Ecosystem model development and evaluation. Macroecology, interactions between biogeochemical cycles and both autotrophs and heterotrophs.
3. **Simon Claus**: Coordinates the biology project of EMODnet. Data management in the Belgian NODC, trait and abundance cross-referencing.
4. **Forough Fendereski**: Marine ecologist working on plankton biogeography and on neural networking methods for the definition of marine biomes. Intelligent clustering and interpolation of marine ecosystem data.
5. **Takafumi Hirata**: Detection of plankton functional groups from space / remote sensing. Member of the MAREMIP SSC.
6. **Xabier Irigoien**: Plankton ecology, trophic relations in plankton, climate effects and biodiversity patterns.
7. **Thomas Kiørboe**: Zooplankton traits, quantification of ecosystem services.
8. **Elena Litchman**: Phytoplankton community ecologist, plankton trait data. Interpretation of patterns from first principles and the combination of trait and abundance data.
9. **Yawei Luo**: Ocean nitrogen cycling. Traits and global biogeochemistry of nitrogen fixers. Member of MAREDAT
10. **Maria Deng Palomares**: Fish population dynamics and fish data. Coordinator of SeaLifeBase, which aims to provide a 'FishBase-like' database for all other marine organisms that are not included in fish databases.

7.2. Associate Members

1. **Andrew Barton**: Ecosystem modeler and trait ecologist. Global marine lower trophic level trait data, combination of abundance and trait data.
2. **Karine Leblanc**: Marine biology with a focus on diatoms and biogeochemical flux measurements.
3. **Stephane Pesant**: Plankton ecology, editor for biological data at PANGAEA, and advocate for citation, open access and reuse of scientific data. Stephane is a member of Tara Oceans, SeaDataNet, and EMODNet Biology, and was guest editor for MAREDAT 2012 Atlas.
4. **Ralf Schiebel**: Foraminifera and palaeoceanography. Long-term changes in marine ecosystem structure and functioning, with a focus on calcifying organisms.

8. Relationship to other international programs and SCOR Working groups

The proposed working group would allow knowledge transfer from SCOR working groups 125 (Global Comparisons of Zooplankton Time Series) and 137 (Patterns of Phytoplankton Dynamics in Coastal Ecosystems: Comparative Analysis of Time Series Observation), but it would focus on open ocean and global scale patterns of both autotrophic and heterotrophic constituents of lower trophic level ecosystems, and the combination of different data types. We will work closely with the World Register of Marine Species (WoRMS), in particular for the review of ecological and biological trait information that is being coordinated in the European Marine Observation and Data Network (EMODnet). We will work closely with ICSU's World Data System, in particular with its thematic data center PANGAEA, where the MAREDAT atlases are published. Biogeographic data published at PANGAEA are cross-linked with registers for taxonomy (WoRMS) and are served/disseminated to SeaDataNet, GBIF, OBIS and EMODNet. The working group would facilitate data exchange on marine planktonic traits, presence/absence data, and methodologies to interrogate the databases to define biogeographies ecological niches and to quantify functional diversity.

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Appendix. Full Member Publications

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Radioactivity in the Ocean, 5 decades later (RiO5)

Working Group proposal to the Scientific Committee on Oceanic Research (SCOR)

Summary Abstract

Over the past 50 years, natural and anthropogenic radionuclides have been instrumental in addressing many important questions in oceanographic research. Yet knowledge gaps remain regarding their spatial and depth distributions and the temporal evolution of many radionuclides of importance to both oceanographic and human health issues. The Fukushima Dai-ichi disaster has also recently heightened public and policy concerns related to the human health effects of radioactivity attributable to external exposure from ocean contact and internal exposure from seafood consumption. The timing is thus right for a new SCOR Working group- "Radioactivity in the Ocean, 5 decades later". The goals of RiO5 are to synthesize in a series of papers, the latest scientific insights that have been gained from new global databases on natural and artificial radionuclide distributions, and to identify gaps in our current understanding and scientific knowledge of marine radionuclides. We also plan to create an online compilation of papers and lectures related to radioactivity in the marine environment that will assist in the education and training of the next generation of marine radiochemists and radioecologists. At the same time, we will develop tools to enhance public understanding of radioactivity. Finally, we will assist in the organization of an international symposium that would bring together academic, nuclear power industry and national laboratory experts working in this area.

Scientific Background and Rationale

The very first SCOR Working Group #1, entitled Radioactivity in the Ocean, was formed in 1958 and met in 1959. Chaired by the Japanese scientist, Dr. Yasuo Miyake, the primary objectives of WG1 were to standardize and improve analytical methods and coordinate world-wide measurements of artificial radioactivity. Indeed, when referring to radioactivity, most still focus on the immediate detrimental impacts of anthropogenic radiation and issues related to contamination. Yet since that time, there has been considerable advancement in the field of marine radioactivity, not only in the measurement and application of artificial radionuclides, but also of cosmogenic and U-Th series radionuclides to study ocean processes. Several SCOR WGs have taken advantage of these advances, such as in the use of thorium-234 as a particle export tracer (WG#116) and radium isotopes in the study of submarine groundwater discharge (WG#112). Many other radionuclides are instrumental in geochronology (^{210}Pb, ^{14}C, ^{137}Cs) or in studies on present and past ocean circulation (^{3}H, ^{129}I, ^{230}Th/^{231}Pa). Regardless of the application, it is necessary to understand: i) the evolution of radionuclide sources (both natural and anthropogenic) over a range of temporal and spatial scales, ii) how to use their inherent geochemistries and decay rates to answer a wide range of oceanographic questions and iii) the potential human health effects of radionuclides in the marine environment.

We propose a SCOR Working Group to look at Radioactivity in the Ocean, 5 decades later (RiO5). RiO5 would provide a comprehensive evaluation of our current knowledge of radioactivity in marine systems. RiO5 would be comprised of an international consortium of radiochemists and ecologists whose major focus will be on increasing scientific and public understanding of the sources, fate, and applications of natural and artificial radionuclides in marine systems. This will be accomplished through updating and improving access to radionuclide databases, providing a synthesis and review of radionuclide distributions, and developing a strategic plan for filling missing knowledge gaps.

The timing is right for RiO5 for many reasons. In the aftermath of the Fukushima Dai-ichi disaster – and after years of relative complacency – the public and policymakers have new, heightened concerns about radioactive contamination and potential human health concerns. We are also still limited by where radioactive wastes may be stored, due to perceived and real threats to environmental safety. Nuclear-fueled ships and submarines ply our oceans. The number of nuclear power plants worldwide (>430) is expanding in many countries and is likely to continue as we replace other forms of power that produce greenhouse gases. There are continued concerns regarding the spread of nuclear weapons and "dirty" bombs. Yet, at the same time, Cold War-era nuclear scientists and radiochemists have retired, creating a need for training the next generation of marine radiochemists and radioecologists. As this is happening, a new global view of natural and artificial radionuclides is emerging through programs such as the SCOR sponsored international GEOTRACES program. Although the isotopes measured by GEOTRACES are a limited set, this is the first such effort since the GEOSECS Program that mapped several radionuclide distributions in the oceans in the 1970's. Indeed, the time elapsed between both major efforts appear as a unique opportunity to examine not only how specific radionuclide inventories have changed, but what those inventory changes mean with regards to their marine geochemistry and implications for global biogeochemical cycles (e.g., Moore et al., 2014).

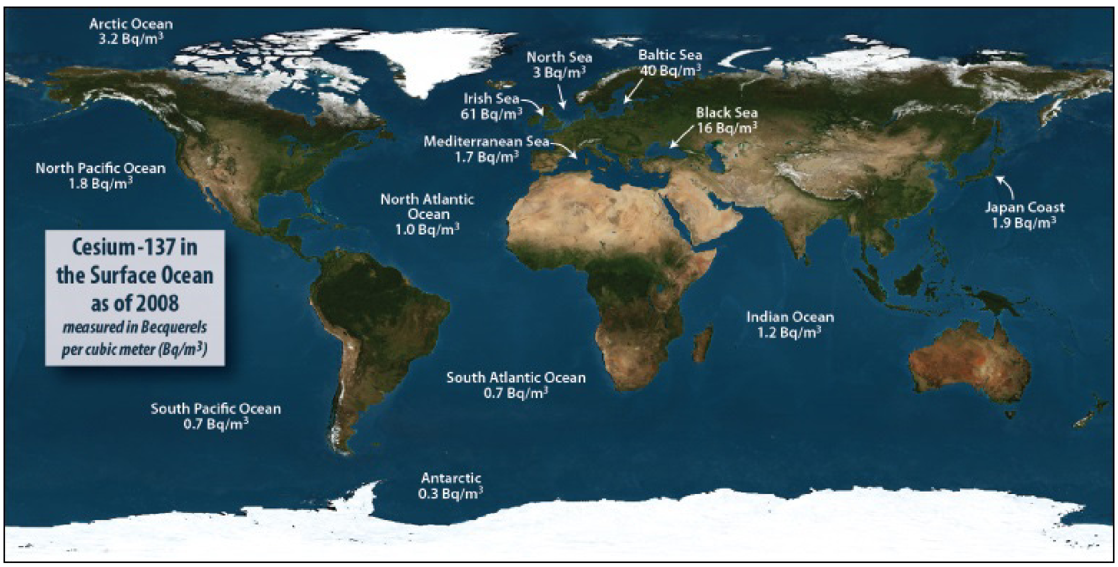

Figure 1. Example of recent compendium of ^{137}Cs activities in marine systems prior to the Fukushima accident. Data source: http://maris.iaea.org Available at: http://ourradioactiveocean.org

One example of the value of such a review of current knowledge is shown here by summarizing the global distribution of ^{137}Cs in the surface ocean (Figure 1). One can immediately observe the following: 1) 1960's fallout ^{137}Cs is rather uniform globally, with slightly higher values in the Northern Hemisphere (due to location of weapons testing) at background levels of 1-2 Bq m^{-3}; 2) higher levels from Chernobyl fallout in the Baltic and Black Seas (20-40 Bq m^{-3}); and 3) perhaps the most surprising, or at least less well known, is that the Irish Sea still maintains the highest ^{137}Cs levels in the ocean due to prior nuclear fuel reprocessing releases from Sellafield. This map further enables the establishment of a baseline for oceanic ^{137}Cs activities prior to Fukushima. In contrast to these levels, ^{137}Cs in the ocean peaked at over 50,000,000 Bq m^{-3} close to the reactors in April 2011 (Buesseler et al., 2012), which was of direct concern to human health and marine biota, and far higher than the concentrations observed after weapons testing or the Chernobyl accident. Three years later, the public remains concerned about the predicted ^{137}Cs activities of 10-30 Bq m^{-3} within the Fukushima plume approaching the west coast of

North America (Rossi et al., 2013). However, these predicted activities are in fact lower than that found today in some of the world's oceans and should not cause any measureable impact on human health. Compilations of global baselines such as that shown in Figure 1 are clearly necessary and allow for such assessments to be made. This and other maps are part of the first steps of RiO5.

Figure 2 is an exciting example of a natural radionuclide data set only recently available online as part of the GEOTRACES Program. While variable and high dissolved ^{210}Pb activities in surface waters are expected due to atmospheric inputs, high activities of ^{210}Pb at depth not only suggest substantial remineralization of sinking particles, but an additional source of ^{210}Pb that has not been previously observed (using mass balance). Such profiles therefore demonstrate how ^{210}Pb may be used to examine sources and cycling of other stable trace elements of similar particle reactivity that are more difficult to assess from their concentrations in seawater.

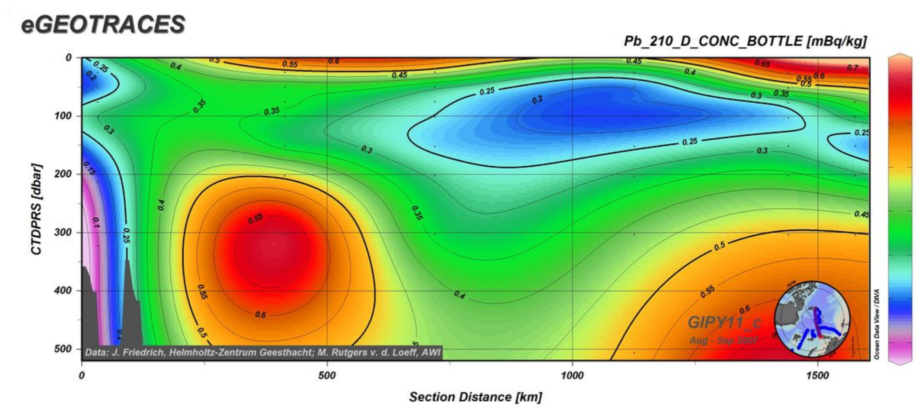

Figure 2. Example of radionuclide data available online as part of the GEOTRACES Program. Data source http://www.egeotraces.org/

A final example showing the strength of pairing natural and artificial radionuclides is from Charette et al. (2014), who used ^{224}Ra as an indicator of coastal water ages (time since contact with sediments and/or groundwater) and found that in samples collected in 2013, the activities of ^{137}Cs near the coast of Japan remained higher than those offshore, similar to ^{224}Ra. Using a mass balance approach they estimated that continued release of ^{137}Cs from the Fukushima NPP site must be occurring (9 GBq per day), a key unknown in the ongoing evaluation of Fukushima ocean impacts.

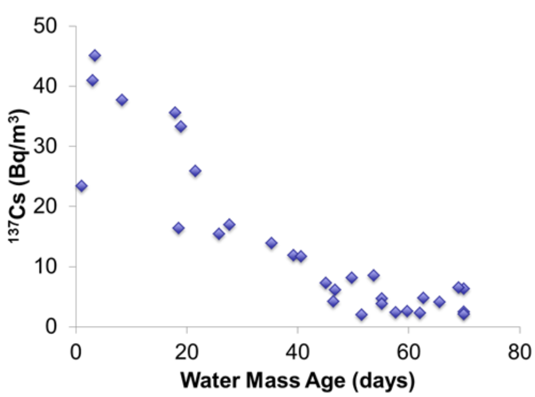

Figure 3. Plot of water mass age derived using ^{224}Ra versus ^{137}Cs activity off the coast of Japan. Source: Charette et al., 2014

These examples illustrate the breadth of new insights obtainable by synthesizing current radionuclide data sets (Figure 1); exploring new features in global transects (Figure 2); and combining studies that include both natural and artificial radionuclides (Figure 3). In addition, tremendous technological developments over the past decade have enabled the measurement of natural and artificial radionuclides at previously unattainable levels. This has revolutionized the radiochemistry field and has been instrumental in discovering new applications of radionuclides to address many important questions in oceanographic research.

RiO5 will bring experts together to review the current knowledge of radioactivity in marine systems and explore and identify research areas where new uses of radionuclides as tracers will be instrumental. These processes include: 1) understanding the global ocean carbon cycle with regards to sources of carbon to marine systems (gas exchange, riverine and ground water, hydrothermal vents, etc.) , *in situ* cycling (nutrient turnover), the transport of material from the surface ocean to depth (biological pump-mediated particle export and remineralization), and burial in marine sediments (months to millennia); 2) understanding ocean circulation in current and paleo climates from coastal ocean currents to large-scale tele-connections between various ocean basins; and 3) understanding contaminant sources, transport and removal of not only the radionuclides themselves, but other elements of similar chemistries, such as bioactive and particle reactive trace elements measured in the GEOTRACES program, some of which have their own pollution concerns (Pb, Hg, Cu, etc.).

Terms of Reference

We propose that SCOR establish a working group called "Radioactivity in the Ocean, 5 decades later (RiO5)" with the following terms of reference:

1. Combine and build upon existing global and individual databases of natural and artificial radionuclide distributions to make an user friendly and easily accessible on line product;
2. Summarize and publish review papers on these global radionuclide datasets and provide examples of how these can help improve our understanding of ocean processes and contaminant fate and transport;
3. Identify gaps in scientific knowledge in relation to radioactivity in the marine environment;
4. Bring together academic, nuclear industry and national laboratory expertise for an international symposium on radionuclides in the ocean;
5. Provide a warehouse of education materials to assist in the education and training of the next generation of marine radiochemists and radioecologists;
6. Develop tools to enhance public understanding of radioactivity, in particular in the ocean.

These activities would be achieved by convening WG meetings (1 per year for 3 years), exchanges among WG Members, building web-based informational resources, writing scientific manuscripts, and finding resources and partners for hosting a large international symposium.

Working plan

This Working Group is envisioned as a three-year activity that we hope will have a legacy beyond the funded study, to create a trusted resource for the ocean sciences and environmental community on matters related to radioactive substances, sources, and wastes in the oceans. The time-line delineated below outlines the major steps and their order to reach the deliverables (see below) according to the defined terms of reference. The timeline does not include much of the between-meeting activities and communications that are important to keep the WG going, which will be the responsibility of the two co-chairs to maintain.

Year 1

WG meeting #1- hosted by M. Dai, Xiamen U. (partial financial support in place through Xiamen U.). In conjunction with WG meeting, a two-day training workshop will be considered as part of the WG capacity building efforts (see Capacity Building below).

- Charge to WG participants- gather information on existing and ongoing radionuclide data bases, such as Marine Information System (MARiS) (IAEA- Morris lead), HAM (Japan- Aoyama lead) and GEOTRACES (Schlitzer Associate Member lead). Use Ocean Data View tools for visualization and use these data to develop global distribution maps (see Figure 2 as example)
- Outline synthetic papers to present the current state of the global oceans for natural and artificial radionuclides, based on the combined datasets achieved above. Spatial distributions and evolution as well as a global overview of potential risk will be the focus of the artificial radionuclide datasets, while objectives for naturally occurring radionuclides include their relevancy with regards to applications and newly available tools
- Discuss challenges and frontiers in marine radiochemistry and radioecology
- Discuss plans for WG web site and how to expand and build and disseminate education materials for public and students. Use WHOI's Center for Marine and Environmental Radioactivity site as host and model of similar activities (http://www.whoi.edu/cmer ; web site costs supported by CMER)
- Introduce plans for an international symposium on marine radioactivity. Decades ago, similar efforts were hosted by UK (MAFF) and French (IRSN) ministries in Cherbourg in 1996 (Radionuclides: a tool in Oceanography 1987; Radionuclides in the Ocean- RADOC 96). IAEA has been approached to help support and host the symposium and welcomes additional discussion upon SCOR funding of this WG

Year 2

WG meeting #2- hosted by K. Buesseler (WHOI meeting facilities support in place); possible alternative is to hold in conjunction with international meeting such as Ocean Sciences to increase participation by Associate Members.

- Review progress done on the database efforts
- Review synthesis papers and prepare for publication
- Develop list of future challenge and areas of need
- Planning for international symposium on Radionuclides in the Ocean, including promotion and organizing co-sponsorship
- Review education and public outreach materials and discuss submission of e-lectures, fact brochures, hands on activities for primary and secondary education and coordinating ongoing hands-on training by various international groups of the next generation of radiochemists

Year 3

WG meeting #3- in conjunction with international symposium.

- International Symposium- collect extended abstracts & manuscripts
- Post conference publication/book and organize associated papers in open access format such as a **Frontiers Research Topic** (http://www.frontiersin.org/blog/What_is_a_Frontiers_Research_Topic_/620)
- Final preparation of wide release of educational materials- for both student and public audiences

Deliverables

1. Connect all available data bases via the IAEA's MARiS portal, including data collected via the GEOTRACES and HAM data bases and individual studies. MARiS is a publicly accessible database in the same spirit embraced by GEOTRACES (http://www.egeotraces.org/) and various time-series programs (HOT (http://hahana.soest.hawaii.edu/hot/hot-dogs/interface.html), PAPA (http://oceanobservatories.org/infrastructure/ooi-station-map/station-papa/), etc.) (WG Members lead: Morris, Aoyama, Masque; Associate Member: Schlitzer)

2. Review papers on ocean radionuclide distributions and future challenges in their measurement and application. (All WG Members)

3. Production of education tools at the primary school, undergraduate, and graduate level. This includes eLectures (http://www.aslo.org/lectures/), online course materials based on courses already being taught by SCOR WG Members (e.g. Johnson, 2014)

4. Public communication and dissemination (web tools and fact sheets) that include basic information on radiation literacy and marine radioactivity using lessons learned from Fukushima to motivate and attract attention (see example at http://www.ourradioactiveocean.org/) (WG Members lead: Benitez-Nelson, Masqué, Buesseler; Associate Member: Johnson)

5. International symposium in year 3 - Radionuclides and Marine Processes – attended by academia, industry, national laboratories, with published scientific abstracts, following the model of the MARC Applications of Radioanalytical Chemistry Conferences. Seek partnership with IAEA (WG Member- Morris) and other EU sponsors (WG Members lead: Oughton, Charmasson, Delfanti) and US private foundations (WG Members lead: Buesseler, Benitez-Nelson)

Capacity Building

Members will participate individually and collectively in efforts to increase public and scientific understanding of marine radioactivity and radioecology. This SCOR WG will seek financial support as needed from the national agencies of WG Members, international organizations like the IAEA and IOC/UNESCO and groups such as, IUR, etc. and private funding sources. By developing tools for web based training, the next generation of graduate students will be exposed more readily to the concepts needed to understand radioactivity and radioecology in the marine environment. By increasing interactions among WG Members and knowledge of national programs, student exchanges and mentoring and sampling opportunities will be enhanced. With web-based sources to promote public understanding about radioactivity and open-access publication of synthesis papers and symposium volumes, there will be new resources to help expand the field and provide information to the public and policy makers.

Activities will include the web-based education materials and documents as well as online courses explained above. But more specifically, RiO5 will also work to-

- Coordinate short term training of both junior and senior researchers at WG Member laboratories
- Facilitate participation of young researchers in oceanographic cruises to be trained in sampling and analyses
- Seek and facilitate appropriate ways of funding for young researchers, for attending research conferences, short-term stays at research centers or PhD or postdoc fellowships
- Approach the IAEA for Technical Cooperation for developing countries. Some of RiO5 Members already collaborate with the IAEA on this and the WG can work with the IAEA to identify future requirements for capacity building
- Pursue capacity building for developing country scientists through participation of developing country scientists in WG, holding first meeting in China in conjunction with a two-day training workshop, and seeking assistance from SCOR to involve participation of developing country scientists in WG activities
- Routine activities of outreach activities are also anticipated through national and regional user groups, such as COSEE China (China Ocean Science Education Excellence Partnership) which is officed at Xiamen U.

Working Group Members

Full Members of this Working Group were selected based upon their scientific contributions, participation in educational activities, leadership as evidenced by participation and chairing national and international committees and symposium, editorships, career awards and recognition, experience in launching new initiatives and a willingness to participate in public and policy discussions on important issues related to marine radioactivity and radioecology. Proposed WG Members were also chosen to be widely representative of international expertise in the field and to span a range of skills and knowledge in marine radiochemistry and radioecology. Associate Members were considered important to expanding that scientific and regional expertise, and will be invited when possible to join us at WG meetings and will be called upon between meetings to assist with specific WG deliverables, as needed.

Full Members

Name	**Gender**	**Place of Work**	**Expertise**
Ken Buesseler*	M	WHOI, USA	Marine radiochemistry, C cycle, public education, GEOTRACES
Minhan Dai*	M	Xiamen U., China	Coastal biogeochemistry, radionuclide applications, GEOTRACES
Michio Aoyama	M	Fukushima U., Japan	Marine radiochemistry, global nutrient cycling
Claudia Benitez-Nelson	F	U. So. Carolina, USA	Marine radiochemistry, methods and teaching

Sabine Charmasson	F	IRSN, France	Radioecology of natural and artificial radionuclides
Roberta Delfanti	F	ENEA, Italy	Radionuclides as ocean tracers of physical processes
Pere Masqué	M	UAB, Spain	Environmental radioactivity and nuclear physics, GEOTRACES
Paul Morris	M	IAEA, Monaco	Radium and thorium isotopes and radionuclide databases
Deborah Oughton	F	NMBU, Norway	Radioecology and radioecological risk assessments
John Smith	M	BIO, Canada	Radionuclides in Arctic and other basins

* = co-chairs

Associate Members			
Andy Johnson	M	Black Hills State Univ., USA	Teaching radiation literacy
Reiner Schlitzer	M	AWI, Germany	Data management and visualization, GEOTRACES database lead
Gary Hancock	M	CSIRO Australia	Soil erosion and sediment transport
José Godoy	M	PUC, Rio de Janeiro, Brazil	Ra, Po, Pb isotopes and groundwater discharge
Nuria Casacuberta	F	ETH, Switzerland	Sr, U and other radionuclide tracers
Jordi Vives i Batlle	M	SKC-CEN, Belgium	Radioecology and radiological protection
Vladimer Maderich	M	Inst. of MMSP, Ukraine	Radioactivity dispersion and fate models
Sandor Muslow	M	ICML, U. Austral de Chile	Radiotracers, stable isotopes and benthic ecology

Working Group contributions

While all Members will participate in all activities of the group, a short description of each full WG Member's unique professional activities and interests, as well as contribution to the WG is provided below.

Ken Buesseler specializes in the study of natural and artificial radionuclides in the ocean and their application to better understanding ocean processes. He will serve as co-Chair of the WG. He leads the Center for Marine and Environmental Radioactivity, the goals of which include increasing scientific and public understanding of radioactive substances in the environment, and training the next generation of marine nuclear radiation experts - all are key components of the RiO5 mission. Buesseler chaired SCOR WG 116 on Sediment Trap and ^{234}Th Methods for Carbon Export Flux Determination.

Minhan Dai uses a suite of radionuclides to examine carbon and trace metal biogeochemistry in marginal seas and estuarine systems, and investigates the geochemistry of radioactive elements in surface and ground water. He will serve as WG co-Chair and contribute by promoting links to research and radioecology in China and in Southeast Asia and will host a WG meeting at Xiamen University.

Michio Aoyama works on the geochemistry of ^{137}Cs in the world ocean from global fallout, and nuclear power plant accidents and has developed a marine radioactivity database, HAM, for artificial radioactivity in the world ocean. He will contribute by further developing and linking current databases of artificial radionuclides in marine systems.

Claudia Benitez-Nelson is an expert in the development of new radiochemical techniques and in the application of short-lived naturally and artificially occurring radionuclides in Marine Systems. A gifted teacher and mentor who has received numerous accolades for her ability to communicate her science to the broader community, she will contribute by coordinating the writing of the overview manuscripts and in the development of classroom and broader public education and outreach materials.

Sabine Charmasson's field of expertise is mainly radioecology with use of both natural and artificial radionuclides as tracers of transfer processes within ecosystems (primarily land-to-sea fluxes, sediment recording, food chain transfer). She will contribute by promoting links with EC research and radioecology, in the development of education and training tools, and with public dissemination.

Roberta Delfanti's research uses radionuclides as tracers of marine processes, including water dynamics in the Mediterranean Sea, and sedimentation and bioturbation in coastal and deep-sea environments. She will contribute by promoting links with eastern European research and radioecology, as well as education, training and public dissemination.

Pere Masqué's research focuses on using both natural and artificial radionuclides as tracers of processes in the ocean at various time scales, from present to paleooceanographic. A former member of the scientific steering committee of GEOTRACES, he will contribute by coordinating database efforts and in the development of education and outreach materials.

Paul Morris has worked with natural radionuclides to study ocean processes such as particle export and mixing rates. Currently, Morris works for the IAEA as the manager and coordinator of the Agency's Marine Information System (MARiS), and will contribute by further developing and linking current MARiS to other emerging data bases on artificial and natural radionuclides in marine systems.

Deborah Oughton's research includes the use of radioactive isotopes as environmental tracers as well as socio-ethical aspects of radiation risk assessment and stakeholder engagement. She will contribute by promoting links with EC research and radioecology, as well as education, training and public dissemination.

John N. Smith carries out targeted research focusing on applications of radioactive tracers to studies of sedimentation and particle transport, fish growth and other biological processes, biogeochemical cycling, ocean circulation and climate change. He will contribute by promoting links with North American research and radioecology, as well as education, training and public dissemination.

Relationship to other international programs and SCOR Working groups

We outline briefly below, some of the agencies and groups we have already spoken to, who will have a role to play in our WG activities. It is important to note that none of these organizations or groups have programs that would replace the need for RiO5, but they all can assist in those efforts in some way.

International Atomic Energy Agency (IAEA) and its Environment Laboratories in Monaco

One of the IAEA's mandates is to advise and assist Member States in building capacity for measurement and assessment of radionuclides in the marine environment and tracer applications to oceanographic, climate-related and pollution studies. Through its Marine Laboratories in Monaco (http://www.iaea.org/monaco/page.php?page=10) the IAEA is the world's major producer of reference materials of marine origin, and organizer of interlaboratory comparisons and proficiency tests. The IAEA maintains the MARiS database, containing over 120,000 records on radionuclides in seawater, marine sediment, and biota. Also, the WG co-Chairs are in discussions regarding an International Symposium with the IAEA, which, pending funding and approval, may be in a position to collaborate through dedicated sessions at a larger conference on nuclear applications in the marine environment.

European Nuclear Safety Training and Tutoring Institute (ENSTTI)

ENSTTI (http://www.enstti.eu/) was founded in 2011 and offers applied training course and tutoring sessions in nuclear safety, nuclear security and human and environmental radiation protection. On this latter point links could be developed with RiO5 in order to provide ENSTTI with baseline studies worldwide, to underline various processes that may enhance radionuclide transfer in the marine environment, even to contribute to ENSTTI training course on marine radioactivity and radioecology.

Center for Marine and Environmental Radioactivity (CMER)

CMER (http://www.whoi.edu/cmer) was established in early 2013 at the Woods Hole Oceanographic Institution with the goals of increasing scientific and public understanding of the sources, fate, and consequences of radioactive substances in the environment, and training the next generation of marine nuclear radiation experts. CMER will host this SCOR WG web site at WHOI, and assist in making links to public, student and academic audiences, building upon several efforts to pass on lessons learned from Fukushima, such as the *Oceanus* (http://www.whoi.edu/page.do?pid=83397&tid=3622&cid=175809) Japanese/English issue- *Fukushima and the ocean*- as well as a highly visited FAQ site (http://www.whoi.edu/page.do?pid=83397&tid=3622&cid=94989) on Fukushima ocean impacts. Also CMER can help organize and co-sponsor one of the WG meetings at WHOI.

Center for Environmental Radioactivity (CRAD)

CERAD (http://www.umb.no/cerad) is a Norwegian funded center of excellence hosted by the Norwegian University of Life Sciences and covering research and education on the sources, transfer, effects and risk assessment of radionuclides in the environment. In addition to fundamental research they are also engaged in stakeholder engagement and policy public issues. They are members of the Radioecology Alliance, and EC projects STAR, COMET, NERIS, DoReMi and OPERRA. They will contribute to training and education activities and links with EU radioecology and radiation protection

International Union of Radioecology (IUR)

The IUR (http://www.iur-uir.org/en) is an independent, non-political and non-profit scientific organization. Its first overarching role is to perpetuate a "think tank" capacity on radioecology issues through the maintenance of a network of scientists and professionals from around the world to foster communication between researchers from different fields and geographical regions through brain storming in task groups, the publication and circulation of technical papers, organization of conferences, training courses, and job alerts. At present there is no marine radioactivity task group, and this is something that RIO5 would be able to promote within IUR, and would be to the benefit of both organizations.

GEOTRACES

GEOTRACES (http://www.geotraces.org/) is an international and SCOR supported effort to map global distributions of selected trace elements and isotopes of key interest in ocean sciences. Two WG Members (Dai and Masque) are former members of the international GEOTRACES SSC, and Associate Member Schlitzer, is leading database efforts that we hope to incorporate into our WG to produce added-value to the efforts underway as part of this program.

Other collaborations

In addition to these groups, we will build relationships through our Full and Associate Members with a wider range of organizations, programs and working groups. Included among these are the Intergovernmental Oceanographic Commission (IOC-UNESCO) (http://ioc-unesco.org/) and the European ALLIANCE (http://www.er-alliance.org/) network and associated COMET and STAR consortiums. These groups will help to identify appropriate ways to ensure and facilitate the accomplishment of RiO5 objectives, including the training of new researchers in the field. European RiO5 WG Members will be proactive in raising funds for training thorough adequate platforms and instruments such as EU-funded Marie Curie Training Networks and/or COST-Actions (European Cooperation in Science and Technology), on which they already have experience.

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SCOR Working Group Proposal

Title: **Designing a biological observing system in the Southern Ocean to inform global ocean observing of marine ecosystems.**

Acronym: **SO-eEOV WG**

Summary/Abstract

Sustained biological observing of marine ecosystems is necessary for developing realistic scenarios of change in species, foodwebs and ecosystems and the attribution of change to their causes. This capability is essential for ecosystem-based management and for developing mitigation and/or adaptation strategies in the long-term. Investment in sustained biological observations requires demonstration that those observations are likely to contribute to detection and/or attribution of change. Current work in the Global Ocean Observing System (GOOS) and the Southern Ocean Observing System (SOOS) has identified many candidate 'ecosystem Essential Ocean Variables' (eEOVs) for long term observations. The comparative simplicity of the Southern Ocean ecosystem and the small number of human pressures compared to elsewhere makes this a useful experimental system for informing the development of biological observing for other more impacted and complex regions. This Working Group will significantly contribute to science of marine ecosystems by designing field programs to acquire data necessary to make scenarios of their dynamics realistic. It will do this by developing tools, procedures and experience from the Southern Ocean; specifically it will (1) assess whether candidate eEOVs will correctly indicate dynamics and/or change in ecosystems of the Southern Ocean, taking into account the potential confounding effects of fishing and global change, (2) evaluate the spatial and temporal sampling requirements, and their concomitant costs, of field observations needed to robustly estimate the candidate eEOVs in the Southern Ocean, and (3) disseminate the tools, framework and outcomes for supporting the design of ecosystem observing systems.

Scientific Background and Rationale

Realistic scenarios of change are a major challenge for marine science (see IPCC Working Group II Assessment Review 5, 2014), making it difficult to place research on the ecology of marine ecosystems in a realistic regional and/or global context. Knowledge of the magnitude and rate at which marine ecosystems are changing is fundamentally important for managing human activities that may affect ecosystem services (e.g., Millennium Ecosystem Assessment, 2005), either through short-term tactical adjustments to keep them sustainable, such as in fishing, or in strategic long-term planning for mitigation or adaptation to long-term change, as for managing climate change. Currently available indicators relate to the physical environment or, for biology, only particular aspects of the ecosystem, such as biogeochemistry or foodweb components affected by fishing (Shin and Shannon 2010).

Assessing biological change requires a sufficiently long time series that allows differentiation of change from natural variability. To date ecosystem indicators have been derived opportunistically from available datasets (e.g., Coll *et al.*, 2009; Cury & Christensen, 2005; Perry *et al.*, 2010). This work suggests that indicators need to be better designed for correctly detecting change and that the observation system needs to be capable of detecting change when it occurs (Constable, 2011; Perry *et al.*, 2010).

The development of sustained biological observing programs for marine ecosystems has received much attention since the Ocean Observing conference in 2009 that led to the Framework on Ocean Observing (FOO; Lindstrom *et al.*, 2012), with activities in the Global Ocean Observing System (GOOS)(First Technical Expert Workshop for the GOOS Biology and Ecosystem, and GOOS Biogeochemistry Panels, November 2013, Townsville, Australia), GOOS Deep Ocean Observing System, and Group on Earth Observations Biodiversity Observation Network (GEOBON). These activities and the recent workshop sponsored by the ICSU, SCOR and SCAR and the Southern Ocean Observing System (SOOS) held at Rutgers University in March 2014 (Constable *et al.*, 2014; hereafter termed 'the Rutgers worskhop') have identified biological variables that could be candidates for being 'ecosystem Essential Ocean Variables' as intended under FOO (Constable *et al.*, 2014). A key challenge that has not been resolved by any biological observing system is to demonstrate which candidate eEOVs need to be given priority for investment in the long-term, i.e. that their state of readiness is mature (sensu Lindstrom *et al.*, 2012). It is widely recognised that the state of readiness of many, if not most, biological variables is currently at the conceptual or pilot stage rather than mature.

An important task is to establish observing systems that can detect change. A second task is to establish and identify those observations that will enable attribution of change to specific causes, probably with the assistance of models. In this case, long-term measurements will be needed to make the dynamics of these models realistic, so that the relative importance of different drivers can be correctly interpreted. A third task is to take measurements that help combine historical datasets, thereby facilitating historical reconstructions to better understand current status and trends of key species and the ecosystem overall.

The set of field measurements to be taken in a biological observing system need to contribute to estimating eEOVs that will further these three tasks; eEOVs have been further defined at the Rutgers Workshop as essential biological or ecological quantities that reflect ecosystem properties – primary productivity, food web productivity, abundance, diversity, energy transfer and global and regional human pressures (Constable *et al.*, 2014). How can the maturity of an eEOV be judged in advance of its long-term implementation?

For the first task on 'detecting change', candidate eEOVs need field measurements that enable signals of change to be detectable above the variability of the system and the noise of measurement error. In this case, datasets that indicate spatial and temporal variation in measurements can be used as a foundation for evaluating two attributes of the eEOVs. The first attribute is whether the eEOV is likely to give a clear signal related to the possible drivers of change, such as whether a change in krill predator reproductive performance can be clearly attributed to change in the abundance of krill (de la Mare & Constable, 2000). Current uncertainties in ecosystem structure and dynamics may mean that differences in the eEOV over time may be difficult to interpret. The second attribute is whether the field sampling design is feasible in space and time to unambiguously yield the expected signal above the background variability. The inclusion of a candidate eEOV in the observing system will be contingent on the quality (interpretation) of the signal and the cost of obtaining that signal.

The second task is to provide measurements that will facilitate tuning models to be realistic in order to investigate change in unmeasurable parts of the system and the attribution of change to particular drivers. In this case, eEOVs do not necessarily need to detect change but provide the foundation for ensuring the dynamics of the model, in terms of the ecosystem properties identified above, are realistic. Sufficient representative (not all) eEOVs at critical times and locations will be needed to capture the dynamic properties of the ecosystem, including the covariance of different components of the system.

Historical datasets may include some eEOVs that will enable ecosystem reconstruction from these datasets. The third task, will be to capture the covariance between critical ecosystem properties and such historical datasets. This covariance will enable hindcasting of ecosystem models by estimating the historical ecosystem properties from these historical time series.

For many candidate eEOVs, field data that demonstrate their variability in space and time already exist. These eEOVs could be progressed to maturity if the requirements for the spatial and temporal design of the field measurements can be evaluated and tested. Data for the eEOVs, synoptic data, such as satellite and ocean model data, and ecosystem simulations can be used to determine how well the candidate eEOVs will generate unambiguous signals for ecosystem properties (change, ecosystem dynamics or covariance with historical datasets) and the cost to deliver those signals.

A SCOR Working Group in collaboration with other international groups, including the IMBER program's Integrating Climate and Ecosystem Dynamics (ICED) in the Southern Ocean, the Southern Ocean Observing System (SOOS), and the Global Ocean Observing System (GOOS), will provide an important vehicle to bring together the international scientific community to evaluate the readiness of candidate eEOVs in advance of their implementation, the latter of which will require long-term commitment and investment in sustained biological observations. The relative simplicity of the Southern Ocean ecosystem and the small number of current human pressures compared to elsewhere makes this a useful experimental system for informing the development of biological observing in other more complicated regions. Furthermore, compared to other global oceans, all regional human pressures in the Southern Ocean are reported, measured and managed through the regulatory bodies. Moreover, considerable progress has been achieved in developing individual methods for sampling Southern Ocean ecosystems (Agnew, 1997; Rintoul *et al.*, 2011) and for modelling these ecosystems (Murphy *et al.*, 2012). A large body of experience is available for assessing change in many marine ecosystems (Perry *et al.*, 2010; Shin & Shannon, 2010). Together, this experience can be harnessed to evaluate the readiness of candidate eEOVs (signal and the cost of field implementation) in the Southern Ocean Observing System. The procedures and results of this work can then inform the development of eEOVs in the GOOS and other observing systems, including organisations developing methods to assess the state of marine ecosystems.

Terms of Reference

The proposed Working Group will:

1. Assess whether candidate 'ecosystem Essential Ocean Variables' (eEOVs) will contribute to making ecosystem scenarios realistic by reliably indicating dynamics and/or change in ecosystems of the Southern Ocean, taking into account the potential confounding effects of fishing and global change.
2. Evaluate the sampling requirements in space and time, and their concomitant costs, of field observations needed to robustly estimate the candidate eEOVs in the Southern Ocean.
3. Disseminate the tools, framework and outcomes for supporting the design of ecosystem observing systems.

Working plan

The Terms of References will be achieved between 2015 and 2017, through coordinated modelling work and data analysis, workshops in South Africa (November 2015) and in the Republic of Korea (November 2016), and a larger symposium to be hosted in China to facilitate greater community involvement (September 2017).

Milestone 1: Assessment of the reliability of candidate eEOVs to indicate ecosystem dynamics and/or change in Southern Ocean ecosystems (November 2015).

Prognoses for change in Southern Ocean ecosystems have been summarised in Constable *et al*. (in press) and Nymand-Larsen *et al*. (2014). The IMBER Program ICED has developed models to represent these ecosystems (Murphy *et al.*, 2012) and determined future scenarios for investigating climate change impacts on the Southern Ocean (Cavanagh *et al*., in prep). The models and scenarios will be used to assess the degree to which uncertainty in ecosystem structure and dynamics may affect signals from candidate eEOVs in the future.

Candidate eEOVs will be those derived from the Rutgers Workshop on eEOVs in the Southern Ocean (Constable *et al.*, 2014); approximately 25 eEOVs have been identified, including those related to the CCAMLR Ecosystem Monitoring Program, to measure change in krill and krill predators, and for estimating the dynamics and trends in Southern Ocean food webs under climate change scenarios. eEOVs identified by GOOS will also be considered.

Work to assess the performance of candidate eEOVs will involve fine-tuning the models to achieve this task as well as developing appropriate metrics of ecosystem states and eEOVs, including methods to visualise and simplify potentially complex results, the latter of which are not currently available. The Working Group will monitor progress quarterly and provide feedback to expert teams established for different sectors of the Southern Ocean, in order to account for regional differences in the ecosystem.

Results will be integrated at the 2015 workshop with the aim of establishing which eEOVs could be classed as having *pilot* readiness, i.e. which candidate eEOVs could reliably indicate dynamics and/or change despite uncertainties and/or variability. The Working Group will then publish the tools and experience in the assessment of candidate eEOVs making them available to other researchers developing eEOVs for their marine ecosystems.

Milestone 2: Evaluation of the design and cost of field programs for measuring the pilot eEOVs (November 2017).

Realistic options for field designs will be determined by using existing data to characterise pilot eEOVs, including time series of *in situ* variables (west Antarctic Peninsula, Scotia Sea), satellite products and model re-analyses. These data and statistical analyses will be used to determine alternative spatial and temporal field sampling designs for measurements underpinning those eEOVs. These methods have not yet been developed for foodwebs and will be an important output of this Working Group. The approach will be discussed at the first workshop and will be undertaken over Year 2 of the Working Group.

A realistic design will need to take adequate account of the spatial and temporal variability that is likely to occur with field measurements. This work will identify the tradeoffs between the cost of the field design and the signal derived for the eEOV.

Prior to the next step, the ecosystem models will be refined so that they can report simulated field observations to support the eEOVs at realistic biological, spatial and temporal scales as well as incorporating possible measurement errors given the field conditions and methods. Methods to downscale ecosystem models to the level of field measurements will be developed in Year 2.

Next, ecosystem simulations of the future scenarios will be used to evaluate the performance and cost of the candidate field designs in the long-term. Performance of the eEOV in these simulations will be judged by how well the eEOV (estimated from the simulated measurements) compares to the actual quantity in the simulated ecosystem. This approach is similar to methods used to evaluate fisheries management strategies (Constable, 2011). These simulations will be used to optimise the quality of the signal relative to the cost of the field program for estimating the eEOVs into the future. The results will be used to determine which eEOVs are feasible and whether they could be regarded as mature and thus be included in the biological observing system. This work will be undertaken over Years 2 and 3.

The workshop in November 2016 will review progress and finalise papers from Milestone 1 and the first part of Milestone 2. This workshop will also be a major planning meeting for the symposium in September 2017, which will review all the outcomes of Milestone 2 and disseminate the experience and results.

Milestone 3: Develop an implementation plan for eEOVs determined to be at a mature stage of readiness and disseminate the experience, tools and products from the work of the Working Group (November 2017).

A Symposium on 'eEOVs and the design of biological observing systems' will be held in September 2017 to share the experience of this Working Group and to finalise an implementation plan for eEOVs for the Southern Ocean Observing System. The state of readiness of the other candidate eEOVs will be reviewed and advice provided on how they might be progressed to maturity. This symposium will have broad participation, which will include presentations on related works, along with a presentation of the candidate eEOVs and the associated design for field implementation of those eEOVs the working group regarded as mature. This symposium is designed to build capacity in biological ocean observing by bringing together experts involved in the work of this Working Group as well as from other national and international marine biological observing initiatives, particularly GOOS.

Deliverables

The third term of reference aims to provide outputs that are useful to other bodies who are also designing marine biological observing systems. These outputs will include:

i) ecosystem models used for evaluating whether signals (dynamics and/or change) arising from eEOVs will be robust to uncertainties in ecosystem structure and function;
ii) statistical methods developed for estimating eEOVs from field observations;
iii) tools and methods for utilising satellite and model data to evaluate the variability in estimates of eEOVs;
iv) methods and routines for downscaling large-scale ecosystem models to report on simulated measurements from the observing system;
v) a final report and consequent scientific publications in an open access journal on the evaluated performance of eEOVs for Southern Ocean ecosystems and their advantages (signal, sampling efficiencies) and disadvantages (cost of sampling, variability/noise); and
vi) an implementation plan for the biological theme of the SOOS.

These products will be made available to GOOS, IMBER, CCAMLR and other organisations interested in developing ecosystem observing systems, as well as to the general scientific community, through the SOOS website (www.soos.aq) and Southern Ocean Knowledge and Information wiki (www.soki.aq). Progress reports and product announcements will also be published regularly through the online SOOS newsletter, to ensure dissemination to the greater ocean observing community.

Capacity Building

An established need in marine ecosystem research is the capability for statistical and dynamic modelling of marine ecosystems. This Working Group will link key expert groups in both Southern Ocean and global ecosystem modelling to enhance existing capability to make ecosystem models realistic and useful for evaluating the design of field programs. The Working Group also has four full Members from developing nations that will provide important opportunities for building capacity in marine ecosystem modelling and approaches to the development of efficient sustained biological observing systems that could be applied to their local situations. In addition to this, the uptake by developing nations of consistent field sampling plans will help their observing efforts gain more leverage internationally, and have greater scientific and societal impact. Both workshops and the Symposium will be held in developing nations, which will further the sharing of skills and building partnerships between research groups in developed and developing nations. The Symposium is also intended to be an open event, and additional funds will be sought to support the attendance of developing country scientists where possible.

The expert groups for each milestone and Southern Ocean region will provide opportunities to build teams of researchers and post-graduate students around each combination of milestone and region. Support for these teams will be provided through ICED, CLIOTOP, SOOS and SCAR. This increased capability will further the objectives of IMBER and the Future Earth program. This Working Group will also contribute to an improved capability for evaluating climate change impacts on ecosystems and will be timely for the sixth assessment review by the IPCC.

SCOR will be approached for extra funding to involve additional developing country scientists in working group activities, beyond those who are Full members of the working group.

Working Group composition

This Working Group requires expertise in observing marine ecosystems, ecosystem modelling and statistics. The Working Group is designed to provide this expertise while achieving the desired discipline, geographical and gender balances. It has an emphasis on building capacity in developing nations in marine ecosystem research and observing.

Full Members

Name	Gender	Place of work	Expertise relevant to proposal
1 Parli Bhaskar	Male	National Center for Antarctic and Ocean Research, India	Microbial ecology, biogeochemistry, Field and Laboratory studies. SOOS
2 Andrew Constable (co-chair)	Male	Australian Antarctic Division, Australia	Modelling, theoretical ecology, field observing. SOOS, ICED, CCAMLR
3 Dan Costa (co-chair)	Male	University of California Santa Cruz, USA	Marine mammal/bird ecology and bioenergetics, field observing measurements. SOOS, ICED, CLIOTOP
4 Katja Fennel	Female	Dalhousie University, Canada	Biogeochemistry, modelling. GOOS, OTN, IMBER
5 Beth Fulton	Female	CSIRO, Australia	End-to-end ecosystem modelling, theoretical ecology, field observing. PICES
6 Eileen Hofmann	Female	Old Dominion University, USA	Biophysical modelling. IMBER, ICED
7 Xianshi Jin	Male	Yellow Sea Fisheries Research Institute, China	Ecosystems/fisheries ecology, Field observing. PICES Fishery Science Committee
8 Olivier Maury	Male	University of Cape Town, South Africa	Ecosystem modelling. ICED, CLIOTOP
9 Monica Muelbert	Female	Universidade Federal do Rio Grande, Brazil	Habitat and population ecology, field observing. IWC, SORP, CLIOTOP
10 Yunne-Jai Shin	Female	Institut de Recherche pour le Développement, France	Ecosystem modelling, ecosystem indicators. IndiSeas Co-convenor

Associate Member

Name	Gender	Place of work	Expertise relevant to proposal
1 Sanae Chiba	Female	Japan Agency for Marine-Earth Science and Technology, Japan	SAHFOS, North Pacific ecosystems
2 Simon Jennings	Male	Centre for Environment, Fisheries and Aquaculture Science, UK	Ecosystem observing, fisheries, macroecology, survey design, indicators, food webs. ICES
3 Bettina Meyer	Female	Alfred Wegner Institute, Germany	Krill observations, systems ecology, Weddell Sea. CCAMLR
4 Eugene Murphy	Male	British Antarctic Survey, UK	Scotia Arc, Ecosystem observing, theoretical ecology, modelling. ICED.
5 Olav Rune Godoe	Male	Institute of Marine Research, Norway	Acoustic observations, ecosystem ecology, Scotia Arc, CCAMLR
6 Ian Salter	Male	University of Bremen, Germany	Microbial ecology, biogeochemical time-series. GOOS-DOOS, SOMLIT
7 Oscar Schofield	Male	Rutgers University, USA	Ecosystem observing, Palmer LTER. SOOS
8 Hung-Chul Shin	Male	KOPRI, Republic of Korea	Southern Ocean ecosystem ecology, CCAMLR
9 Sandy Thomalla	Female	CSIR, Republic of South Africa	Oceanography, Biogeochemistry, ocean observing. SOCCO
10 George Watters	Male	AMLR Program USA	Ecosystem observing, modelling. US AMLR, CCAMLR

Acronyms:

CCAMLR (Commission for the Conservation of Antarctic Marine Living Resources)
CLIOTOP (IMBER - Climate Impacts on Oceanic Top Predators)
GOOS-DOOS (GOOS Deep Ocean Observing System)
ICED (IMBER - Integrating Climate and Ecosystem Dynamics in the Southern Ocean)
ICES (International Council for the Exploration of the Sea)
IMBER (Integrated Marine Biogeochemistry and Ecosystem Research)

IWC (International Whaling Commission)
LTER (Long Term Ecological Research)
OTN (Ocean Tracking Network)
PICES (North Pacific Marine Science Organisation)
SAHFOS CPR (Sir Alistair Hardy Foundation for Ocean Science)
SOCCO (Southern Ocean Carbon and Climate Observatory)
SORP (Southern Ocean Research Partnership of the IWC)
SSC (Science Steering Committee)
US-AMLR (USA program on Antarctic Marine Living Resources)

Working Group contributions

Parli Bhaskar has background in microbial processes and food-web dynamics (especially the microbial loop), in the Indian and Southern Oceans. He will contribute to field standardisation, evaluation and implementation of candidate eEOVs at lower trophic levels.

Andrew Constable (co-chair) is a theoretical ecologist using ecosystem models to assess the effects of climate change and fisheries on Southern Ocean ecosystems and is Vice-chair (Biology) of SOOS SSC. He will use his models and statistics to help standardise and evaluate eEOVs.

Dan Costa (co-chair) has extensive experience on the foraging ecology and movement of top predators in the Southern Ocean and the North Pacific and Bering Sea, is on the SCAR Expert Group on Birds and Marine Mammals, and SOOS, ICED and CLIOTOP SSCs. He has pioneered the use of animals to obtain oceanographic measurements and will provide expertise in obtaining data from animals about their movement and environment.

Katja Fennel has expertise in regional coupled physical-biological modelling and assimilation of biological and biogeochemical data. She will focus on modelling of ecosystem processes at lower trophic levels (i.e. phytoplankton and zooplankton dynamics), assimilation of observations and evaluation of observing system design.

Beth Fulton has extensive global experience in whole-system modelling (developer of Atlantis), leading teams to evaluate management and monitoring/observing strategies in marine ecosystems around the world. She and her team will use end-to-end ecosystem models to test the theoretical performance of different eEOVs and indicators and explore the information costs and benefits of alternative monitoring schemes.

Eileen Hofmann brings experience in modelling physical-biological interactions in marine ecosystems, with particular focus on the Southern Ocean and is Chair of the IMBER SSC and co-convenor of ICED SSC. She will contribute expertise on identifying eEOVs that are needed for development, calibration and evaluation using marine ecosystem models constructed for Southern Ocean systems.

Xianshi Jin is an expert in the ecology of ecosystems, including variability of ecosystem structure and high trophic level dynamics. He will contribute to the standardisation of eEOVs and their measurement, including field evaluations and implementation of eEOVs at high trophic levels.

Olivier Maury is on the CLIOTOP SSC and has worked to assess climate change impacts on top predators, particularly through development of size-based food web models (APECOSM). He will adapt APECOSM to the Southern Ocean to undertake simulation experiments to identify which variables would be critical to observe to characterise ecosystem variability, and to assess eEOVs on whether they properly characterise ecosystem states.

Monica Muelbert is on the SCAR Expert Group on Birds and Marine Mammals and is a key investigator in Brazil on tracking of marine mammals. She will provide the working group with expertise in population dynamics, genetics and tracking of higher predators in South America.

Yunne-Jai Shin is an IndiSeas co-convenor with end-to-end ecosystem modelling expertise (developer of OSMOSE) as well as expertise in the analysis of ecosystem indicators. She will use her ecosystem models to test the theoretical performance of different eEOVs, as well as the development of methods to analyse eEOVs from field data.

Relationship to other international programs and SCOR Working groups

This topic is of fundamental theoretical importance to marine science as well as management, which are key goals for SCOR. SCOR already has experience in providing leadership in the development of indicators through its Working Group 119 (Cury & Christensen, 2005), which provided foundations for further work on fisheries indicators, e.g. IndiSeas (Shin & Shannon, 2010) and PICES (Perry *et al.*, 2010), and Working Group 125, which considered trends in zooplankton. Also, SCOR has current working groups considering time series of phytoplankton (Working Group 137) and methods for developing time series of the chemical environment (Working Group 143), which together will provide important inputs to whole-ecosystem indicators and monitoring. The involvement of SCOR will provide the impetus for engaging with the wider community on this issue, including scientists from academic and government institutions as well as young researchers and those from developing countries.

Marine ecosystem management will require indicators of the underlying status of marine ecosystems and how they may be changing, such as is highlighted by the UN World Oceans Assessment whose first assessment is scheduled to be delivered in 2014 (the Regular Process for global reporting and assessment of the state of the marine environment, including socieconomic aspects, St. Aimee & Sauvé, 2011). Marine ecosystem indicators will also inform the science for assessment cycles of the emerging Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services (IPBES), as a parallel to the IPCC. However, development of such indicators is not far advanced, particularly whole-ecosystem indicators. Experts involved in these panels have become involved in discussions on eEOVs prior to the Rutgers workshop and will be engaged with the process of their evaluation.

Recent attention to the development of field programs to measure change on large ecosystem scales has recognised deficiencies in understanding what biological parameters may be routinely measured to provide effective indication of the trajectories of change of those ecosystems (Murphy *et al.*, 2008; Rintoul *et al.*, 2011). In particular, there is a growing recognition of the need to measure the background state of ecosystems to facilitate interpretation of indicators from fisheries, for example, the IndiSeas Working Group of the Eur-Oceans Network of Excellence (Shin & Shannon, 2010), the North Pacific Marine Science Organization (PICES) assessment of the North Pacific marine ecosystem status (Jamieson *et al.*, 2010), and in the Scientific Committee for the Conservation of Antarctic Marine Living Resources (SC-CAMLR) (SC-CAMLR, 2011). The delivery of biological observing systems and support modelling and statistical tools relevant to these organisations has been a focus of GOOS, GEOBON and SOOS, ICED, SCAR, and IMBER amongst others. Products arising from this Working Group will be provided to all these organisations through the Working Group Members that participate in these respective bodies.

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Appendix

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Optimized design of an ocean observing system for biogeochemistry in a changing climate

1. Summary

While great strides have been made in ocean observing technology over the last decades, the ocean remains significantly under-sampled with respect to biogeochemistry. However, there is mounting evidence that the ocean is currently undergoing detectable changes and is not in steady state, with this having the potential to alter the ocean's future role in not only carbon uptake, but also the rates and locations of ocean acidification, the supply of oxygen to ocean ecosystems, and the availability of nutrients to fuel ecosystems and fisheries.

Concurrent advances in ocean biogeochemical models have facilitated the development of Observing System Simulation Experiments (OSSEs). OSSEs allow one to assess the skill of observing systems in identifying target signals. The goal of this Working Group is to make recommendations for optimal observing system design through combined consideration of observing platforms and state-of-the-art models.

2. Scientific Background and Rationale

In light of the public awareness and urgency of monitoring the oceans, the oceanographic biogeochemistry and ecosystem communities have articulated a number of key questions:

- (A) How is the ocean uptake and storage of carbon distributed in time and space? Is it changing?
- (B) What are the climatological structures of net community production (NCP), export production (EP), and primary production (PP) in the ocean?
- (C) What are the climatological structures of ecosystem stressors in the ocean, including ocean de-oxygenation and the saturation state of aragonite (Ω_{arag})? And how are these changing in time?
- (D) How do the principal biological provinces evolve in time? And how are they modulated by the subduction and obduction of nutrients within the ocean?

A variety of methods have been developed to characterize the evolving ocean uptake of carbon, making use of both interior inventory changes and global air-sea fluxes inferred from surface pCO_2 data, and the suite of methods applied in the RECCAP efforts of the Global Carbon Project. The results from the RECCAP efforts revealed that for much of the global ocean, large discrepancies remain at all but the largest spatial and temporal scales among the different techniques used to estimate carbon uptake.

For productivity, community efforts have led to the development of climatologies for Net Community Production (NCP), Export Production (EP), and Net Primary Productivity (NPP), and time-varying NPP products from satellite data. Ocean biological provinces have been characterized through a variety of methods that synthesize a broad range of constraints (*Sarmiento et al.*, 2004). Combined use of time-series data and repeat hydrographic measurements has facilitated the characterization of the ocean climatology, as well as trends in ocean de-oxygenation and acidification.

Each of the above goals still faces challenges associated with data/sampling sparsity issues of the current observing system. One such challenge is temporal bias given the tendency for most ship-board measurements to be made in summer. Another is spatial bias clearly encompassing the sparse coverage over many regions of the Southern Hemisphere. It is also important to consider that many of the successes in monitoring with the existing observing network have relied heavily on surface measurements, including those relying on pCO_2 and remote sensing products. An emerging conceptual framework of using ocean water masses to understand biogeochemical provinces and ecosystems has begun to emerge, but to date this approach has tended to focus on models due to lack of seasonal coverage. Additionally, the current CMIP5 generation of Earth System Models indicates that biogeochemical provinces aren't stationary and will be impacted by shifting gyre boundaries and water mass structures (*Bopp et al.*, 2001; *Sarmiento et al.*, 2004; *Bopp et al.*, 2013). Importantly, these questions are largely interrelated since ecosystem patterns are tightly connected to biogeochemical processes as well as to the 3-D structure of the ocean circulation. Given this inter-relatedness, and the potentially high cost of expanding the observing system, it is critical to consider ways to optimize the observing system.

Our goal in proposing a SCOR Working group is to develop an integrated view of observing system design that will optimally sample the ocean to address the needs of the community. Our interests as a Working Group span the four questions detailed above, although given the time constraints and scope of a SCOR Working Group our priorities will be on the first two. The observational challenges of answering these questions will clearly benefit from assessment of a shared multi-platform observing network, with a number of the essential ocean variables being common to our central priorities. A critically important goal in optimizing the observing network will be the specification of quantitative thresholds for detection of the fields described above, and to optimize the observing system to balance the needs of the community. It would of course be advantageous to define such thresholds for specific variables measured (T, S, DIC, nutrients, etc.) rather than for the more abstract concepts listed above. This will benefit from work that has already been conducted to define Essential Ocean Variables (EOVs) for physics, biogeochemistry, and ecosystems. Sampling strategies for these variables can then make use of Observing System Simulation Experiments (OSSEs) with state-of-the-art forced ocean model runs. For OSSEs, the full evolving state of the model can be assessed to round-off precision, and strategies for observing system design can be tested. Of course all of the caveats involved with using models will need to be considered as well.

This type of strategy has already been investigated with OSSEs for the case of carbon uptake by the ocean (item "A" above), where the Large Scale CO_2 Observing Plan (LSCOP) of *Bender et al.* (2002) prescribed 10% uncertainty in net carbon uptake as an upper bound for the target accuracy of the Repeat Hydrography network. This has been considered by *Plancherel et al.* (2013) for the case of uptake of anthropogenic carbon over the North Atlantic between the 1990s and 2000s (WOCE-to-CLIVAR), where it was argued that the Repeat Hydrography network should be capable of detecting decadal trends to within 10%. This strategy was also considered for the case of monitoring pCO_2 (and thereby air-sea fluxes of CO_2) over the Southern Ocean by *Majkut et al.* (2014). There an idealized representation of floats measuring pCO_2 was used to argue that 200 floats could be sufficient to monitor decadal trends in air-sea CO_2 fluxes. The non-eddying ocean model configurations used in these studies provide a useful first platform for iterative interactions with the observational community, and it is expected that models will benefit greatly from this interaction.

If an uncertainty threshold of 10% is considered appropriate for the other variables of interest, the current ocean observing system is insufficient. Although important work has been done in characterizing decadal trends in ocean interior O_2, we are not yet able to construct a global monthly climatology of O_2 in the upper ocean to within uncertainties of 10%. Clearly, even greater challenges lie in developing monthly climatologies for NCP, PP, and EP over the global ocean within a 10% threshold. The question naturally arises, if one begins by specifying an uncertainty threshold, what would be the optimal path for expanding the current observing system in order to achieve this goal? In addressing this question, it is important to consider water masses as a unifying framework for ocean biogeochemistry (*Walin*, 1981; *Iudicone et al.*, 2011), and their value in the interpretation of data. The importance of water masses to classifications of biomes is already implicit in the study of *Sarmiento et al.* (2004), through the upwelling and subduction patterns over large scales.

2.1 Overview of target signals and tools

The central objective here is to recommend an optimally designed ocean observing system for addressing the science objectives listed at the head of this document. The system will need to be expanded to satisfy simultaneously the needs of physical, biogeochemical, and ecosystems communities, while at the same time integrating with and adding value to existing observing system elements such as Argo.

Through activities of the GOOS Framework for Ocean Observing (*Task Team for an Integrated Framework for Sustained Ocean Observing*, 2012), efforts are now underway to address a number of related objectives for ocean observing, including:

(1) To define a suite of Essential Ocean Variables (EOVs) for physics, biogeochemistry, and ecosystems for both scientific and resource management (monitoring) considerations
(2) To coordinate observing networks that contribute to the EOVs, including issues of standards, data sharing, and developing metrics etc.
(3) To coordinate with partner organizations to reach a consensus data model for EOVs
(4) To propose pilot projects for expansion of the observing network.

Although the larger objectives pertain to the science and resource management questions described above, the quantitative assessment of network design will hinge on measurements of a suite of Essential Ocean Variables (EOVs). We intend to build upon the recommendations provided by GOOS panels and advisory groups, themselves drawing on international expertise, in articulating the target variables and necessary sampling resolution for the expansion of the observing network.

The overarching goal of the Working Group will be to make a series of recommendations for pilot projects, as well more general recommendations for optimized design of the ocean observing system. Equally importantly, the group will also draw on the recommendations of GOOS panels in recommending a suite of unified EOVs for both the pilot projects and the global observing network. The recommendations will be focused on determining the optimal network design needed to address the set of community-shared scientific and monitoring priorities detailed at the head of this document. In other words, what is needed to achieve the high priority scientific goals listed above? What are the estimated costs?

Efforts to better quantify productivity (NCP, PP, and EP) will be important to both carbon cycle and ecosystems research, and improved estimates will be contingent on seasonally resolving, three-dimensional measurements. Important efforts have already been made to characterize these quantities through the use of remote sensing products. However, in the absence of seasonally varying subsurface fields, quantifying uncertainty associated with these fields has proven elusive. Thus, for the suite of biogeochemical and physical EOVs needed to characterize NCP, PP, and EP, the precision threshold should be ~10%. In addition to proposing optimal EOVs for monitoring the carbonate system in the ocean, *our goal will be to recommend strategies to detect global surface ocean trends, and to characterize thresholds for detection. It will be important to decide whether the 10% threshold is appropriate more generally, or whether a less stringent threshold of 20% or 25% would be appropriate.*

Even with a perfect observing system, there is also the ever-present question of whether measured decadal trends can be interpreted as the secular anthropogenic climate signal, or to what extent natural variability is included. For example, this question has been raised concerning the current decadal hiatus in global surface temperatures representing a pause in a trend towards global warming (*Meehl et al.*, 2011). In this context, it is useful to consider uncertainties associated with the observing system itself as "systematic uncertainty", and uncertainties associated with natural variability as "random uncertainty". Modeling efforts such as *Henson et al*. (2010) and *Henson et al*. (2013) have sought to address detection of secular trends in the presence of natural variability.

All of this needs to be considered within the context of the multi-platform observing system described above.

2.2 Modeling issues

Global ocean biogeochemical models have grown in sophistication over the last decade. Two commonly used classes of ocean-only models are used widely, (a) state estimates that assimilate observations such as the ECCO and SODA models, and (b) forward models such as MOM and NEMO. Although models are and will continue to be 'works in progress', they have demonstrated value in testing observing system design through Observing System Simulation Experiments (OSSEs).

Progress has been made in understanding the relationship between biogeochemical processes and water masses in the ocean (*Iudicone et al.*, 2011), and this has been complemented by important efforts with eddy-permitting models to better understand water mass transformation processes (*Nishikawa et al.,* 2013). The large-scale structures of biogeochemical properties are prescribed by the interplay between biological, chemical and thermodynamical processes and are thus best understood in terms of water masses. This three-dimensional dynamical view of the oceans needs to be coupled with ensembles of processes on seasonal and interannual time scales that further contribute to setting ocean properties in the photic zone. For example, the monitoring of nutrients in the interior has to be complemented by a characterization of the interplay between nutrient availability at the surface (as set by local physical and biological processes), and interior distributions via subduction-related processes and even non-local controls of surface processes (where obduction occurs). Important steps towards understanding the interplay between surface and interior processes have been taken (e.g., *Palter et al.*, 2005). Again, this is considered to set the context for the Working Group activities, which will be specifically focused on the observing network.

3. Terms of Reference

The main goals of the Working Group will be to make recommendations that fall into three general categories. The first will be to characterize the ocean biogeochemical state from the existing network. The second will be to articulate an appropriate suite of Essential Ocean Variables (EOVs) building on and extending the work of GOOS advisory groups and other experts, as well as to consider detection thresholds and OSSE design. The third and fourth will be focused on recommendations for pilot studies and on optimization of the global observing network. These questions will be considered within the context of the newly available technology, such as biogeochemical sensors for profiling floats and gliders, and complementing the existing global platforms such as Argo and remote sensing products.

4. Working Plan

4.1 Task Set #1: Characterize the ocean biogeochemical state from existing network

The first task set will involve a careful evaluation and review of what can be inferred from the existing observing network. Here we will identify 'state-of-the-art' estimates as those that have appeared in the peer-reviewed scientific literature.

(i) What is the optimal combination of Essential Ocean Variables (EOVs) for meeting the needs of communities monitoring physical oceanography, ocean biogeochemistry, and ocean ecosystems?
(ii) What estimates exist for the rate at which carbon is being absorbed by the global ocean?
(iii) What quantified estimates exist for biological productivity, and what are the associated uncertainties in current estimates of PP, NCP, and EP?
(iv) What is understood about the important ecosystem stressors, including ocean de-oxygenation and acidification parameters?
(v) What is the state-of-the-art for ocean biogeochemical modeling?

4.2 Task Set #2: Define detection thresholds and OSSE design

The second task set will focus on a synthesis of the candidate target variables and multiple-platform optimization:

(i) Refine and specify the target suite of Essential Ocean Variables (EOVs), incorporating the lists provided by the advisory panels to GOOS;
(ii) Refine and specify precision thresholds for these EOVs, both for climatological and secular trends;
(iii) Recommend a suite of models and conceptual tools that will be appropriate to the OSSE design;
(iv) Set a list of priorities as requirements for a unified OSSE design. It will be important to assess, for example, the degree to which winter under-sampling biases can be reduced with no cost through re-allocation of resources used for summer sampling.

4.3. Task Set #3: Design of pilot studies

The third suite of priorities concerns pilot studies for the observing goals described above. The goal will be to address temporal and spatial sampling issues in regions that are known to be important for the suite of questions listed at the beginning of this document. An important example would be that of subtropical mode waters, whose formation regions are at best severely under-sampled at the present time during winter. In this case one would choose a specific subtropical mode water formation region that can be considered broadly representative, and consider the pertinent spatial and temporal scales for monitoring. In addition to subtropical mode waters, it would be of interest to include regions representative of western and eastern boundary regimes, as well as subpolar and equatorial obduction or re-emergence regimes. Pilot studies will need to directly address the broader question of optimal system design. The important questions will include:

(i) Which dynamical regimes (mode water formations, boundary regions, obduction regions) and what seasons are most poorly constrained with the current observing system, for the suite of EOVs developed through Task Set #1?
(ii) What are representative regions well suited for Pilot Studies? And should a relatively stringent 10% uncertainty threshold be appropriate?
(iii) What pilot studies can help to identify the critical temporal and spatial scales for these regions?

4.4 Task Set #4: Recommendations for optimizing the global observing network

The fourth set of priorities concerns the more general question of the global observing network. This will draw on the recommendations made for OSSEs as well as the recommendations made for pilot studies. The questions to be addressed are:

(i) What is an appropriate uncertainty threshold for the EOVs as part of a global observing network? Would a less stringent threshold for uncertainty (e.g. 20% or 25%) be reasonable on global scales for 3-d fields, and a relatively stringent threshold (e.g. 10%) for surface fields?
(ii) What are the critical scales and processes needed for OSSEs on global scales?
(iii) What are the challenges for an integrated multi-platform OSSE?

5. Working Group Membership, Group Activities, and Capacity Building

5.1 Capacity Building

The members of the Working Group represent a broad international group of researchers with interdisciplinary research experience. In addition to scientific expertise in both observational- and modeling-based research, members of the Working Group have been actively involved in efforts to develop new observing strategies and/or the development and application of Observing System Simulation Experiments (OSSEs). In developing proposals for optimal observing system design, our interests are in building an international effort that builds capacity in developing countries as well as with younger scientists. Our final meeting will be held in a developing country. As two of our Full Members are representing South Africa and Brazil, it is our intention that the final meeting should occur in one of these two countries. It will be our intention with the final meeting to additionally organize a Workshop for two days on Observing System Design, with this meeting open to local participants. Special attention will be devoted to attracting early career scientists to the Workshop.

Full Members

Name	Gender	Place of work	Expertise relevant to proposal
1 Keith Rodgers (co-Chair)	M	US	Global ocean biogeochemical modeling
2 Daniele Iudicone (co-Chair)	M	Italy	Ocean biogeochemical modeling and water mass analysis
3 Toshio Suga (co-Chair)	M	Japan	Large-scale ocean circulation and ventilation processes
4 Moacyr Araújo	M	Brazil	Modeling of ocean circulation and turbulence, and modeling of ocean biogeochemistry
5 Hervé Claustre	M	France	Ocean color; optical oceanography
6 Katja Fennel	F	Canada	Regional biogeochemical modeling; data assimilation
7 Stephanie Henson	F	UK	Biological responses to climate variability and climate change
8 Masao Ishii	M	Japan	Ocean carbon and biogeochemical measurements
9 Eun Young Kwon	F	Korea	Global ocean biogeochemical modeling
10 Marcello Vichi	M	South Africa	Global ocean biogeochemical modeling

Associate Members

Name	Gender	Place of work	Expertise relevant to proposal
1 Claudie Beaulieu	F	UK	Statistical analysis and trend detection
2 Maria Cavanaugh	F	US	Ocean biological provinces
3 Fabrizio d'Ortenzio	M	France	Marine optics and remote sensing
4 Burke Hales	M	US	Ocean biogeochemical measurements
5 Andrew Lenton	M	Australia	Global ocean biogeochemical modeling
6 Sayaka Yasunaka	F	Japan	Variability in carbon and nutrient cycling in the ocean

5.2 Working Group Activities

Annual meetings will be organized by invitation, and will be limited to the members and invited experts to provide summaries of progress and to recommend future directions for the Working Group. We propose that one annual meeting be convened per year during 2015-2017. The first meeting will be in Japan, where Task Sets #1 and #2 will be considered. The second meeting will be conducted in New Orleans to coincide with the 2016 Ocean Sciences meeting, and this will be dedicated to Task Set #3. At the Ocean Sciences meeting, we will also organize a Town Hall meeting. The final meeting, which we intend to have in either South Africa or Brazil, will be dedicated to Task Set #4 as well as a synthesis of the first three Task Sets.

We also intend to develop and submit a paper on Observing System Design to Biogeosciences. Additionally, the suite of recommendations prepared by the group will be made available to the community in the form of reports of the annual meetings.

5.3 Deliverables

The principal deliverables of the Working Group will be consist of the set of recommendations for: a unified set of Essential Ocean Variables, thresholds for detection of these variables, and a suite of of Observing System Simulation Experiments. Additionally we will issue a set of recommendations for pilot studies and for the optimized global network. An additional deliverable will be the review article authored by the members on Observing System Design, to be submitted to Biogeosciences (open access).

6. Working Group Contributions

Here we present the contributions expected from the Full Members. Keith Rodgers' contributions will derive from his experience in using ocean models to interpret ocean biogeochemical measurements, as well as from experience in the design and interpretation of Observing System Simulation Experiments. Daniele Iudicone's contributions will reflect his research efforts to apply water mass transformation analysis to ocean carbon and biogeochemistry. Toshio Suga's contributions will derive from his extensive experience with Argo floats, as well as his extensive research experience involving ocean circulation and ventilation processes. Moacyr Araújo's contribution will stem from his broad interdisciplinary work with both observing system elements and models. Hervé Claustre's contribution to the Working Group will reflect his wide-ranging research into ocean ecosystems, through combined use of multiple elements of the ocean observing network, including Argo. Katja Fennel's contribution will derive from her broad experiences using models to interpret ocean biogeochemical measurements and ocean ecosystems. Stephanie Henson's contribution will result from her experience in trend detection for ocean biology and ecosystems, within the context of climate change, as well as her experience in questions of observing system requirements to detect trends in ocean biology and ecosystems. Masao Ishii's contribution will follow from his extensive work with measuring and interpreting ocean biogeochemistry and acidification trends, as well as through his leadership experience in producing the PACIFICA data product. Eun Young Kwon's contribution will reflect her expertise in modeling both ocean biogeochemistry and ocean ventilation processes. Marcello Vichi's contribution will follow from his extensive experience in modeling ocean biology and ecosystems.

7. Overview of existing SCOR elements

The proposed Working Group will build on the results of previous Working Groups supported through SCOR. In particular, we intend to build on the results of WG 142 focused on Quality Control Procedures for Oxygen and Other Biogeochemical Sensors on Floats and Gliders, as well as on WG 143, on Dissolved N_2O and CH_4 measurements. Interaction with WG 142 will be facilitated that both Hervé Claustre and Katja Fennel (Full Members in our proposal) are members of that WG. If our proposal is supported, we will also contact the co-chairs of WG143 so as to benefit from their work as well.

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Biographical Information

Below is a summary of the contact information, educational background, and pertinent publications for the Full Members of our SCOR Working Group Proposal "Optimized design of an ocean observing system for biogeochemistry in a changing climate".

Full Members:

(1) Keith Rodgers (co-chair)
PhD, 1998 Columbia University, US
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5 pertinent publications:

Rodgers, K.B., J.L. Sarmiento, O. Aumont, C. Crevoisier, C. de Boyer Montégut, and N. Metzl (2008), A wintertime uptake window for anthropogenic CO_2 in the North Pacific, Global Biogeochem. Cycles, 22, GB2020, doi:10.1029/2006GB002920.

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(2) Daniele Iudicone (co-chair)
PhD, 2007, Institute Universitaire Européen de la Mer IUEM
Researcher, Stazione Zoologica Anton Dohrn, Italy
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5 pertinent publications:

Iudicone, D., K.B. Rodgers, I. Stendardo, O. Aumont, G. Madec, L. Bopp, O. Mangoni, and M. Ribera d'Alcala (2011), Water masses as a unifying framework for understanding the Southern Ocean Carbon Cycle, Biogeosciences, 8, 1031-1052.

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(3) Toshio Suga (co-chair)

PhD, 1991, Tohoku University, Japan
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5 pertinent publications:

Oka, E., B. Qiu, S. Kouketsu, K. Uehara, and T. Suga (2012), Decadal seesaw of the Central and Subtropical Mode Water formation associated with the Kuroshio Extension variability, J. Oceanogr., 68, 355-360.

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(4) Moacyr Araújo
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5 pertinent publications:

Brandt, P., M. Araújo, B. Bourles, P. Chang, M. Dengler, W.E. Johns, A. Lazar, C.F. Lumpkin, M.J. McPhaden, P. Nobre, and L. Terray (2013), Tropical Atlantic Climate Experiment (TACE), Exchanges (Hamburg), 18, 26-31.

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5 pertinent publications:

Claustre, H., M. Babin, D. Merien, J. Ras, L. Prieur, S. Dallot, O. Prasil, H. Dousova, and T. Moutin (2005), Toward a taxon-specific parameterization of bio-optical models of primary production: A case study in the North Atlantic, J. Geophys. Res., 110, C07S12, doi:10.1029/2004JC002634.

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(6) Kajta Fennel

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5 pertinent publications:

Fennel, K., J. Hu, A. Laurent, M. Marta-Almeida, and R. Hetland (2013), Sensitivity of hypoxia predictions for the Northern Gulf of Mexico to sediment oxygen consumption and model nesting, Journal of Geophysical Research-Oceans, 118, 990-1002.

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5 pertinent publications:

Henson, S., H. Cole, C. Beaulieu, and A. Yool (2013), The impact of global warming on seasonality of ocean primary production, Biogeosciences, 10(6), 4357-4369.

Beaulieu, C., S.A. Henson, J.L. Sarmiento, J.P. Dunne, S.C. Doney, R.R. Rykaczewski, and L. Bopp (2013), Factors challenging our ability to detect long-term trends in ocean chlorophyll, Biogeosciences, 19(4), 2711-2724.

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5 pertinent publications:

Ishii, M. R.A. Feely, K.B. Rodgers, et al. (2013), Air-sea CO_2 flux in the Pacific Ocean for the period 1990-2009, Biogeosciences, 11, 709-734.

Ishii, M., H.Y. Inoue, T. Midorikawa, S. Saito, T. Tokieda, D. Sasano, A Nakadate, K. Nemoto, N. Metzl, C.S. Wong, and R.A. Feely (2009), Spatial variability and decadal trend of the oceanic CO_2 in the western equatorial Pacific warm/fresh water, Deep-Sea Res. II, 56, 591-606.

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Ishii, M., and HY. Inoue (1995), Air-sea exchange of CO_2 in the central and western equatorial Pacific in 1990, Tellus B, 47, 447-460.

(9) Eun Young Kwon

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5 pertinent publications:

Kwon, E.-Y., S.M. Downes, J.L. Sarmiento, R. Farneti, and C. Deutsch (2013), Role of the seasonal cycle in the subduction rates of upper-Southern Ocean Waters, 43, 1096-1113.

Kwon, E.Y. (2013), Temporal variability of transformation, formation, and subduction rates of upper Southern Ocean waters, J. Geophys. Res. Oceans, 188, 6285-6302, doi:10.1002/2013JC008823.

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Kwon, E.Y., F. Primeau, and J.L. Sarmiento (2009), The impact of remineralization depth on the air-sea carbon balance, Nature Geosciences, 2, 630-635.

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(10) Marcello Vichi
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5 pertinent publications:

Bopp, L. L. Resplandy, J.C. Orr, S.C. Doney, J.P. Dunne, M. Gehlen, P. Halloran, C. Heinze, T. Ilyina, R. Séférian, J. Tjiputra, and M. Vichi (2013), Multiple stressors of ocean ecosystems under global change: projections with CMIP5 models. Biogeosciences, 10, 6225-6245, doi:10.4195/bg-10-6225-2013.

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Vichi, M., A. Navarra, and P.G. Fogli (2013), Adjustment of the natural ocean carbon cycle to negative emission rates, Climatic Change, 118, 105-118.

Vichi, M., J. Allen, S. Masina, and N. Hardman-Mountford (2011), The emergence of ocean biogeochemical provinces: a quantitative assessment and a diagnostic for model evaluation, Global Biogeochem. Cycles, 25, GB2005, doi:10.1092/2010GB003867.

Vichi, M., S. Masina, and F. Nencioli (2008), A process-oriented model study of equatorial Pacific phytoplankton: the role of iron supply and tropical instability waves, Progress in Oceanography, 78, 147-162.

SCOR Working Group Proposal Template
(max. 5000 words, excluding Appendix)

Title:

Rheology, nano/micro-Fluidics and bioFouling in the Oceans.

Acronym:

RheFFO

Summary/Abstract (max. 250 words)

Scientific Background and Rationale (max 1250 words)

The sea is a non-Newtonian biofluid. Yet most oceanographers are still unaware of this, or if they are aware, they do not have the training to apply these findings to their own research and models.

Twentieth-century engineers successfully applied the Derjaguin-Landau-Verwey-Overbeek (DLVO) model of "no wall slip" to fluids in most industrial processes. This model was not designed for plankton. As recent developments in nano- and microfluidics, including "lab-on-a-chip", have shown, surfaces in fluids exert influence from nanometre to millimetre scale into the fluid. (Jenkinson, in press). This is extremely relevant to nano- and microplankton, particularly the micrometre-scale feeding appendages of copepods and other zooplankton.

Encounter and fouling of surfaces by plankton, including their larvae, take place largely in near-surface layers. Recent developments in "green" (i.e. non-toxic) methods of antifouling on ships and other marine structures, can be applied to investigate adhesion, recognition, and repulsion by plankton.

GEOHAB (2011) posed the question, "How can we quantify modifications in turbulence by phytoplankton through changes in the viscosity of its physical environment?" At that time, the state-of-the-art was that viscosity η of seawater and freshwaters was composed of an aquatic component η_W due to water (and salts) plus an excess organic component , η_E due mainly to EPS.

Total viscosity,

$$\eta = \eta_W + \eta_E \qquad \text{[Pa s]} \qquad (1)$$

Broadly, η_E shows a negative relationship power-law relationship with shear rate $\dot{\gamma}$, so that

$$\eta_E = k.\dot{\gamma}^P \qquad \text{[Pa s]} \qquad (2)$$

where k is a coefficient related to EPS concentration and type. P can vary from 0 to ~-1.4 (shear thinning), and has exceptionally been found positive (shear thickening). η_E also varies with phytoplankton concentration. Using chlorophyll *a* concentration *chl* as a proxy for phytoplankton,

$$\eta_E = chl^Q.\dot{\gamma}^P \qquad \text{[Pa s]} \qquad (3)$$

where Q is the phytoplankton concentration exponent, found to about 1.3 generally. Further research, however, has shown the Q can vary locally with the growth phase of the bloom, and even become negative (negative correlation between viscosity and *chl* locally in a *Phaeocystis* bloom) (Seuront et al., 2006). EPS also imparts elasticity to the water. Swimming trajectories of copepods over scales of mm to cm are also greatly changed by viscosity from *Phaeocystis* EPS (Seuront & Vincent, 2008).

EPS thickening, moreover, is generally lumpy; this produces length-scale dependent viscosity, which can be modelled using a lumpiness exponent.

Eq. 3 can now be "corrected" for length scale by a third exponent:

$$\eta_E = k.chl^Q.\dot{\gamma}^P.(L/M)^d \quad \text{[Pa s]} \quad (4)$$

where L is the length-scale of interest, M is the length scale of measurement, and d is the length-scale exponent. A model of whether lumpy EPS could thicken the water enough to stabilize a pycnocline found (Jenkinson & Sun, 2011a) found that the value of d in Eq. 4 was very critical. To investigate d, η of phytoplankton and bacteria (PB) cultures was measured in capillaries of different radii (Jenkinson & Sun, 2014). While η was increased in some combinations of shear rate, capillary radius, 0.35 to 1.5 mm, and PB) species, presumably by EPS, η was reduced in other combinations, including in low Reynolds-number flows, suggesting superhydrophobic drag reduction (SDR) at the surfaces of plankton and or aggregates of exopolymeric substance (EPS). SDR is well known on the surfaces of lotus leaves and many other natural and manufactured surfaces (Rothstein, 2010), where it can be associated with protection against dirt and fouling organisms (Durr & Thomason, 2010), while changing surface electrical fields (Qiu et al., 2011; Wang et al., 2014). These effects are active from nanometres to up to 25 µm (Ou et al., 2004) from surfaces.

Some effects of increased viscosity and elasticity, as well as nano- and microfluidics (NMF) (with suggested primary length scales) include:

	Effect(s)	**References**	**Associated scales**
1.	Damping of turbulence and of sub-Kolmogorov-scale water movement	Jenkinson (1986)	1 nm – 1 m
2	Due to elasticity and lumpiness, complex changes to patterns of water movement, and de-coupling of shear rate from dispersion:	Jenkinson (1986)	1 nm – 1 m
3	Partial and/or total clogging of the gills of fish, molluscs, tunicates, sponges, polychaetes, etc.	Jenkinson (1989), Jenkinson et al. (2007)	1 nm – 1 mm
4	Due to rising organic matter and adsorption to the air-sea surface, reduction of air-sea gas exchange, wave and ripple damping.	Carlson (1987), Calleja et al. (2009)	10 µm – 10 m
5	Complex situations, illustrated by *Phaeocystis*, which produces closely associated stiff mucus holding cells together in colonies, while also producing looser diffuse mucus that increases viscosity at larger scales, as studied in sludge organic aggregates.	Seuront et al. (2006), Liu et al. (2010).	50 µm- 1 m
6	Flocculation into mucous aggregates, thus increasing sinking or rising speed and hence vertical organic flux.	Mari et al. (2012)	a.~100 µm b. up to ~1000 m
7	Reinforcement of pycnoclines by PB EPS	Jenkinson & Sun (2011, 2014)	10 cm-10 m
8	Trapping of toxins close to metabolically active surfaces, such as cell membranes and gills	Jenkinson (1989)	10 nm-1 mm
9	Changes in electrical fields at surfaces of organisms, non-living organic structures and non-organic structures, relative to protection against corrosion, dirt and fouling	Qiu et al. (2011), Wang et al. (2011, 2014).	1 nm-1 mm
10	Changes in viscosity and elasticity by coordinated swimming in plankton	Thutupalli et al (2011)	1 µm- 1 mm

For references, please see both “Key References” and “Members’ Key Publications”.

Investigation techniques of seawater and lakewater to be considered by the *RheFFO* WG include:

Rheology

1. Rheometry: a) concentric cylinder; b) sliding piston; c) capillary flow; d) ichthyoviscometry;

2. Studies of fluid movement at small scale: a) 3D particle image velocimetry (PIV); b) 3D particle tracking velocimetry (PTV);
3. Studies of small forces at small scale: Atomic Force Microscopy (AFM)
4. Combination of electrochemical techniques with rheometry, microscopy and PIV/PTV, ***in situ* if and when possible**;
5. Taking advantage of high biomass in many harmful algae blooms (HABs) to use high-viscosity, marked surface effects and intense cell-cell ecological, physiological, biogeochemical and encounter interactions.

Nano- and microfluidics of biosurfaces (particularly sticking layers and slip layers at surfaces)

6. High-speed video with PIV and PTV of flow through capillaries coated with organic sculptured layers of hydrophobic (Rothstein, 2010), hydrophilic (Bauer & Federle, 2009) and omniphobic (Wong et al., 2011) surfaces. To be combined with transmission electron microscopy (TEM), scanning electron microscopy (SEM), pressure/flow curves, and possibly standard rheometry of the test materials.
7. Scanning electrochemistry of organic matter film dynamics: Hanging mercury drop.
8. Use of electrochemical techniques developed to study the effects of biological coatings on corrosion dynamics;
9. Studies of attraction-repulsion fields, electrical double layers (EDLs).
10. Immunological type radicle-radicle recognition and adhesion.
11. Impact of phytoplankton and EPS on clogging microfiltration apparatus particularly in relation to desalination plants and harmful algal blooms (HABs). (See also following section.)

Biofouling, with adhesion, recognition and repulsion

12. Fouling organisms need to encounter suitable surfaces, recognise them as suitable, then initiate a series of actions to adhere to the surface, and possibly to use means to penetrate it. Organisms subject to fouling are likely to have evolved antifouling mechanisms to avoid being fouled. Related to fouling and antifouling actions can be considered:
    a) Predation and avoidance of predation
    b) Sexual encounter and its defeat;
    c) Parasitism/symbiosis and its defeat;
    d) Pathogenic infection (by bacteria, viruses) and its defeat.

13. Techniques developed largely for “green” biomolecule-modulated industrial antifouling techniques (for ships, cooling intakes, fish-farm cages and nets, etc.) need to be used to investigate fouling of organisms by other organisms and of living and non-living substrates in the sea (plankton, fish and benthic organisms, organic aggregates, sediment, rocks, etc.).
14. Impacts of biofouling and antifouling techniques on clogging of microfilters and its mitigation, particularly in relation to desalination plants.

Rheology modification by co-ordinated swimming

15. Consideration of rheology modification by “swarmers” (Herminghaus, 2011)

Terms of Reference (max. 250 words)

Vision: The ocean science community lacks expertise in (1) Rheology; (2) Nano- and microfluidics; (3) Fouling and antifouling, adhesion, recognition and protection in relation to trophic, sexual, parasitic pathogenic and other types of encounter, that take place close to electrically controlled surfaces including glycocalyxes. Without this knowledge among ocean researchers, modellers and engineers, future models of how the oceans will react ecologically and biogeochemically to future changes will be unnecessarily flawed.

Objectives:

A To create a corps of ocean researchers, modellers and engineers literate in (1) Rheology, (2) Nano- and microfluidics; (3) Fouling and antifouling at surfaces, expertise that they will teach to their students, graduate students and postdocs.

B. During the lifetime of the WG, carry out expert-to-expert interdisciplinary CB and brainstorming sessions, to allow the WG members to carry this expertise to other oceanographic problems, to involve the members' students in theoretical and empirical research, published in scholarly papers, books, multimedia, and incorporated in outreach material across the globe.

Deliverables

See Working Plan below.

Working plan (logical sequence of steps to fulfil terms of reference, with timeline. Max. 1000 words)

Kick-off time, can be discussed with SCOR, perhaps September 2015, OSM in Qingdao in April 2016.

Year	**Actions**
1	To kick off the WG an advanced draft of the RheFFO WG Core Research Programme and Recommendations will be created, by the members before any meeting.. Back-to-back two-day Open Science Meeting and two-day restricted Brainstorming Workshop 1, both held in the Chinese Academy of Sciences, Institute of Oceanology, Qingdao, China. **Six to 12 months from beginning of WG in spring or autumn** **Two-day Open Science Meeting on RheFFO:** Invitations widely disseminated internationally. Anticipated attendance 50-70. Sponsorship sought in Chinese science organizations, city, province and national governments, cultural and scientific organizations, private and public companies. Publication of refereed proceedings in ***Chinese Journal of Oceanology and Limnology*** **(CJOL)** (Ian Jenkinson is Editor in Chief), including summary and conclusions and recommendations paper by the committee of experts. **RheFFO Workshop 1** Immediately following the Open Science Meeting; This is a **Two-day restricted workshop on RheFFO.** (1 day - science reports, discussion and expert-to-expert interdisciplinary CB; 0.5 day writing the summary, conclusions, recommendations; 0.5 day WG organization, and preparation for Year 2). Anticipated attendance 10 (all full members participate.) After the OSM and workshop, the experts will work together to write a paper on a designated aspect of RheFFO, for a high-impact, open-access, scholarly journal, led by designated chair. Decide on time and place of next workshop in about 12 months. Finalise the RheFFO Core Research Programme, with recommendations for future ocean research, CB. Progress report 1 for SCOR leadership.
2	**RheFFO Workshop 2:** time and place decided at previous workshop. All experts participate, with their PGs and PDs as deemed suitable. Anticipates attendance 10 to 20.

	Continued expert-to-expert interdisciplinary CB – One lecture per expert. Decide time and place of next workshop After the workshop, the experts will work together to write a paper on a designated aspect of RheFFO different from that in Year 1, for a high impact open access scholarly journal, led by designated chair. Progress report 2 for SCOR leadership
3	**RheFFO Concluding Workshop 3:** time and place decided at previous workshop. All experts participate, with their PGs and PDs as deemed suitable. Anticipates attendance 15 to 25. Continued expert-to-expert interdisciplinary CB –. One lecture per expert. Decide whether a future workshop is needed, and if so, its time and place. After the present workshop, the experts will work together on a paper on a designated aspect of RheFFO different from that in Years 1 and 2, with overall conclusions for a high impact open access scholarly journal, led by one or two designated chairs. Progress report 3.for SCOR leadership
4	**In Year 4, collaboration will be done by electronic contact, and physical encounters of opportunity, unless a designated meeting is deemed necessary.** All the publications and reports shall be completed or in press by the end of Year 4. Final report of the WG for SCOR leadership. In additional to this final WG report, a final paper for high-level publication will be prepared, that will be a scientific review of new conclusions derived from results obtained by members and others, made during the WG leading to conceptual advances in rheology, nano- and microfluidics, and biofouling, pointing out new questions and gaps in knowledge, and recommendations for future research.

Deliverables (state clearly what products the WG will generate. Should relate to the terms of reference. Max 250 words). A workshop is not a deliverable. Please note that SCOR prefers that publications be in open-access journals.

Proceedings of the Kick-off OSM in Year 1, with 10-20 refereed papers, to be published as a special edition of *Chinese Journal of Oceanology and Limnology.*

1 Kick-off Core research programme for the RheFFO WG

4 papers in top learned journals.

3 annual progress reports

1 Final Report for publication by SCOR.

Capacity Building (How will this WG build long-lasting capacity for practising and understanding this area of marine science globally. Max 500 words)

Capacity building (CB) will be intense in this WG, and partly atypical.

Because the WG will be highly interdisciplinary, initial CB will concentrate on the experts building capacity in each other to produce a world-wide corps of scientists with expertise in rheology, nano- and microfluidics, and biofouling and antifouling, along with the electrochemistry tools to do some of this research, all in relation to plankton ecology, biogeochemistry and other aspects of oceanography. This expert-to-expert CB will continue throughout the WG to progressively deepen interdisciplinary understanding.

In addition, from year 2 to year 4, more classical CB will kick in, with the different experts building interdisciplinary capacity in younger scientists. Interdisciplinary expertise will furthermore be built in these young scientists by teaching and co-mentoring of PDs and PGs by several experts, as well as other exceptional young scientists invited into the WG workshops.

Working Group composition (as table). Divide by Full Members (10 people) and Associate Members, taking note of scientific discipline spread, geographical spread, and gender balance. (max. 500 words)

Full Members (no more than 10, please identify chair(s))

Name	**Gender**	**Place of work**	**Expertise relevant to proposal**
1 Ian R. Jenkinson Initiator, possible chair	M	Chinese Academy of Science Institute of Oceanology, Key Laboratory for Ecology and Environmental Sciences, Shandong, Qingdao, China	Physical-Chemical-Biological coupling, particularly related to plankton. Pioneer on measuring the rheology (viscosity and elasticity) of seawater, particularly in relation to phytoplankton and harmful algal blooms. Rheology and ocean turbulence. Superhydrophobic surfaces. engineering; Early-career research on algal biofouling.
2 Elisa Berdalet Possible chair	F	Institut de Ciències del Mar (CSIC). Pg. Marítim de la Barceloneta, 37-49. Barcelona, Catalunya, Spain	Physical-biological interactions. - Harmful Algal Blooms. - Biochemical methods. - Microplankton physiology. Vice-chair of the Scientific Steering Committee of the SCOR/IOC-UNESCO program GEOHAB, Global Ecology and Oceanography of Harmful Algal Blooms (since 2009).
3 Stephen Herminghaus	M	Max Planck Institute of Dynamics and Self-Organization, Dept. Dynamics of Complex Fluids, Göttingen, Germany	Head of large research group at Max-Planck-Institut. Fields relevant to this WG are dynamics of complex systems, surface effects on deformation, effects of swarmers on liquid rheology.
4 James G. Mitchell Possible chair	M	School of Biological Sciences, University of Flinders, Adelaide, South Australia	His research group consists of 27 people, including postdoctoral fellows and scientific staff from all over the world. Research in his group focuses on the influences of nanometer to micrometer scale processes on marine ecosystems. The ocean is a complex environment on this scale. Lessons they have learned have been applied to nanotechnology, including microfluidics and nanofabrication.
5 Qiu Ri	M	State Key Laboratory for Marine Corrosion and Protection, Luoyang Ship Material Research Institute, Qingdao, Shandong, China	Assistant professor. Research interests are prevention of marine biofouling and corrosion, particularly using “green” organic techniques and surface properties. Superhydrophobic surfaces. Electrochemistry as a tool to measure ion migration and as for changing behaviour of fouling organisms.
6 Laurent Seuront Possible chair	M	Centre National de la Recherche Scientifique,	Phytoplankton, zooplankton, coastal oceanography, multiscaling and

		Laboratoire d'Océanologie et de Géosciences, Université de Sciences et de Technologies de Lille, Station Marine, Wimereux, France.	(multi)fractals in physical, biological and economic systems, and particularly in marine ecology, seawater viscosity in relation to phyto- and bacterioplankton.
7 Peng Wang	M	Chinese Academy of Science Institute of Oceanology, Key Laboratory for Marine Corrosion and Protection, Qingdao, Shandong, China	Assistant professor. Research interests are prevention of marine corrosion and biofouling, particularly using "green" organic techniques and surface properties. Electrochemistry. Superhydrophobic surfaces.

Possibility for adding member(s)

Associate Member (no more than 10)

Name	**Gender**	**Place of work**	**Expertise relevant to proposal**
1 Tim Wyatt	M	CSIC, Institut de Investigaciones marinas, Vigo, Galicia, Spain	HABs, fisheries, organic matter and ecological engineering; eclecticism and excellent writing style.
2 Li ZHUO	F	Tongji University, College of Environmental Science & Engineering, Shanghai, China	

Possibility for adding member(s).

Working Group contributions (max. 500 words)

Detail for each Full Member (max. 2 sentences per member) why she/he is being proposed as a Full Member of the Working Group, what is her/his unique contribution?

BERDALET, Elisa.

1. Elisa Berdalet is an expert on the modulation of the ecology and physiology of different microplankton groups by physico-chemical processes especially at small spatio-temporal scales.
2. She shall contribute to the WG through her experience in biochemistry (including dissolved organic compounds), physiology of phytoplankton and dynamics of harmful algal blooms, as well as using her recent experience of biofouling experiments related to desalination plants.

HERMINGHAUS, Stephen

1. Stephan Herminghaus heads the department 'Dynamics of Complex Fluids' at the Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, that performs research on collective behavior and pattern formation in soft matter systems, which are of central relevance in many geoscience problems, in particular for understanding the dynamics of self-propelled entities, such as some plankton.
2. SH shall provide expertise and guidance in microfluidics, rheology and structure formation in complex matter to the WG, will provide equipment and be instrumental outside the WG for the study of the interaction of active swimmers with the surrounding flow fields.

JENKINSON, Ian R.

1. Ian Jenkinson is a pioneer on measuring the viscoelasticity of seawater and algal cultures, in relation to turbulence and nano- and microfluidics in plankton, as well as to ecology, biogeochemistry and evolution, and he is now a researcher at the Chinese Academy of Science, Qingdao, China, and ACRO, France, as well as journal editor (Oxford University Press, Springer Publications).
2. IJ shall guide the WG particularly in respect to rheological aspects of seawater, and to the composition and subject composition of the WG deliberations.

MITCHELL, James G.
1. James Mitchell specialises in microscale structures and to biodynamic relations, particularly in plankton.
2. JG shall guide the WG in water flow and biodynamics at small scales, as well as in microfluidics and nutrient flux at rough and sculptured surfaces.

QIU, Ri
3. Ri Qiu has been using electrochemical tools to work on marine antifouling based on superhydrophobicity and slippery liquid-infused porous surfaces (SLIPS) for over 5 years, and he has 4 recent publication related to marine fouling and corrosion control.
4. Ri Qiu shall thus guide the WG particularly in relation to surface-based and electrochemically-based control by organisms, both of surface fouling and its defeat.

SEURONT, Laurent
1. L. Seuront is internationally recognized for his expertise in micro-scale patterns and processes in the ocean.
2. LS's 5 recent publications describing (i) the origin of biologically-driven viscosity and its temporal dynamics and (ii) inferring the potential impact of this excess viscosity on structure and function in pelagic ecosystems, shall allow him to guide the WG in relation to bioproduction of excess viscosity, as well as its effects on structure and function in pelagic ecosystems.

WANG, Peng
1. Peng Wang has worked for several years on the effects of superhydrophobic surface structure on modifying electrical fields and reducing corrosion. He is an expert in electrochemistry.
2. PW shall use his expertise for helping the WG to understand biomodification of surfaces and electrical fields at the surfaces of plankton organisms, and shall build capacity in the biologist members of the WG.

Relationship to other international programs and SCOR Working groups (max. 500 words)
- Air-sea exchange, ripple and wave dynamics, air-sea gas exchange, including GLOBEC, SOLAS, WOCE...
- Ocean turbulence programmes, including GOTM, GETM, FABM.
- Programmes related to ocean ecosystem ecology and biogeochemistry, related to global human population and lifestyle, such as IMBER.
- Programmes on dynamics of erosion-and deposition, dredging, etc. of cohesive sediment and fluid mud dynamics.
- Plankton encounter dynamics, trophic dynamics, mating and social dynamics in plankton.
- Programmes in Rheology
- Programmes in nano- and microfluidics.
- Programmes on protection against corrosion and biofouling of ships, aquaculture facilities, and other marine structures.

Key References (max. 500 words)
Please see also "Key Publications" by WG members.

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<u>Appendix</u>

For each Full Member, indicate 5 key publications related to the proposal.

BERDALET, E.

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