The Legacy of \textit{in situ} Iron Enrichments: Data Compilation and Modeling

Introduction

From 1993 onwards there have been 10 \textit{in situ} iron fertilization experiments, from Ironex-1 (1993) to SEEDS-2 (2004), as well as 3 natural fertilization studies (1992 Southern Ocean JGOFS, 2004-2005 Crozex, 2005 KEOPS). Primary results of individual experiments have been reported in \textit{Nature} and \textit{Science} as well as in oceanography journals, sometimes in special issues of journals like \textit{Deep-Sea Research II} and \textit{Progress in Oceanography}. For the most recent experiments (e.g. Eifex 2004, SEEDS-2, CROZEX, KEOPS) primary results are now being processed into manuscripts.

Synthesis of the combined experiments has only just now started with one first semi-quantitative effort by multiple authors (\textit{de Baar et al., 2005}) focusing on only the most basic variables (i.e. primary production, major nutrients, CO$_2$ system variables). This is seen as the modest first step towards more rigorous quantitative assessment by ecosystem simulation modeling of these unique time-series experiments. Nevertheless, several remarkable trends are becoming apparent from the combination of experiments. For example, light limitation due to depth of the wind-mixed layer was highly significant, and the major floristic response was always by larger size class diatoms, with almost universal flourishing of \textit{Pseudonitzschia} sp. Unfortunately, during this first synthesis effort it was found that integrated datasets of even the earlier single experiments of the 1993-2000 period hardly existed, with one laudable exception (SOIREE, data CD in 2001 \textit{DSR-II} special issue). At most, the individual scientists had their own data files which were kindly and generously made available. Sometimes fundamental data (e.g. hydrography, incoming sunlight or PAR) could hardly be traced; some other data of interest could not be located in time vis-à-vis the publication time frame of the synthesis article.

In addition to this synthesis of basic variables of the then-available 8 experiments, there have been some recent articles combining 2-3 experiments for specific topics, that is, CO$_2$ budgeting (\textit{Bakker et al. 2005}) and DMS(P) processes (\textit{Turner et al., 2004}).

A special synthesis workshop (FeAX) was held in Wellington (New Zealand) in November 2005 under the aegis of SOLAS. Currently, the insights gained during that workshop are being written into another, mostly
Rationale

The iron enrichment experiments have been done at great expenditure of scientists’ time, research vessel time, and other costs. Thus overall, taxpayers of various nations worldwide have invested heavily in these experiments. Yet apart from the typical first round of articles on any single experiment, this investment has not led to an international resource or heritage. The already collected but thus far widely scattered data, once brought together, would be extremely valuable for various reasons:

- the ocean science community needs to fully exploit the results of preceding in situ experiments before proposing and implementing the next generation of experiments. In other words, there is no credibility to continue asking taxpayers to subsidize one experiment after another in the future, unless the ocean science community first fully exploits the investments of the past decade. Full use of existing data may yield insights to help design future experiments.

- properly compiled datasets of both natural and in situ iron fertilizations, which will allow the application of 'generic' simulation modeling, thus yielding insights and model robustness far beyond what is feasible by simulating just one experiment. Simulation modeling can include physical mixing, phytoplankton productivity, overall ecosystem functioning, iron chemistry, CO₂ budgeting, DMS(P) processes, and combinations of these variables and processes.

- the value of the experiments is far beyond the ‘iron issue’. For example, the experiences and findings of labeling (SF₆ and sometimes ³H as well) and following a patch of water are most valuable for designing future ‘lagrangian’ experiments for a wide variety of purposes well beyond the iron issue. If nothing else the simulation modeling of dispersion of the added tracer(s) is a learning tool for quantifying lateral and vertical mixing in the surface oceans. Moreover, the practical ability to follow a surface water mass or ‘patch’ over periods of weeks to months allows a wide range of topical biogeochemistry studies.

Objectives

The objectives of the proposed working group are twofold:

1. Data compilation. Assembling a common open-access database of the in situ iron experiments, beginning with the first period (1993-2001; Ironex-1, Ironex-2, SORIE, EisenEx, SEEDS-1) where primary articles have already been published, to be followed by the 2002 experiments where primary articles are now in progress (2002; SOFeX and SERIES), to be followed by the most recent experiments (2004; EIFEX, SEEDS-2). Similarly for the natural fertilizations S.O.JGOFS (1992), CROZEX (2004/2005) and KEOPS (2005).

2. Modeling. Simulation by 'generic' modeling of two or more (2-10) such experiments for various topics such as oceanic mixing processes, plankton ecology, carbon budgeting, and DMS(P) processes.

1. Data compilation

An international Working Group under the aegis of SCOR and with full endorsements by SOLAS and other international bodies is deemed essential for success in compiling all the appropriate databases. At the planning stages of each experiment, mutual access of data is commonly agreed and most funding agencies require the data to enter the public domain within 24-36 months after completion of the granted project. Nevertheless, in practice, compilations beyond individual investigators rarely occur, for a variety of reasons:
Projects tend to be under-funded, often subject to budget cuts before granting, and the originally intended data management often is quietly sacrificed.

At the level of the individual scientist only the most essential data are rapidly picked out for publication of articles, and an individual dataset often is not even compiled.

Some types of data can be produced relatively rapidly, sometimes already available at the end of the cruise, while other types of data require much painstaking labor afterwards in the home laboratory. Physical oceanography data tend to become available for the community at large within 2-3 months, but marine chemists and biologists seem to be far slower in data dissemination.

In summary, our marine science community at the onset of each new project has been intending data management and eventual open access, yet for various reasons in the end this has rarely been accomplished. This proposal aims to remedy this situation for the *in situ* iron enrichment experiments, which may also serve to improve data practice of other future ocean experiments.

An international Working Group will be able to set the example (i) for readily making available data, first to colleagues of the given experiment and next to the open access database, (ii) for proper recognition of the original scientist, (iii) for enhancing the slow culture of one discipline to meet the faster data dissemination practices of another discipline, and (iv) for re-assuring hesitant scientists about protection of their interests as original data producer.

2. **Modeling**

Simulation models pivoting around phytoplankton ecology have thus far been performed independently for SOIREE (Hannon et al., 2001), IronEx (Chai et al., 2002), SEEDS-1 (Yoshie et al., 2005), SERIES (Takeda et al., 2005; Denman et al., in press), and comparison of Ironex-SOIREE-SEEDS (Fujii et al., 2005; Fujii and Chai, submitted). Moreover, there exists a refined simulation model on DMS(P) of SERIES (LeClainche et al., 2006). For physical mixing versus dispersion of SF6 tracer, efforts are being made by Goldson, Law and others. Implications for Ocean Biogeochemical Climate Models (OBCMs) including full ocean circulation and cycling of trace element iron are being pursued by Follows, Sarmiento and others. In general within each class of models, that is, plankton models, mixing models, OBCMs, the individual models vary widely in design and objectives, and much can be learned by comparison between such models.

The Working Group will in a suite of 2-3 workshops bring together these modelers as well as key experimentalists to compare models, define common standard scenarios for validation and, in general, make available the compiled datasets (objective 1.) to the evolving community of modelers.

**Terms of Reference**

Within the proposed 4-year period of existence, the WG plans to achieve the following objectives:

1. Compilation of a database for open access (via the Internet) of the following experiments in three steps:
   1.2. the 2002 experiments (SOFeX-North, SOFeX-South, SERIES)
   1.3. the 2004 experiments (Eifex, SEEDS-2), plus natural fertilizations CROZEX, KEOPS

   This effort will include a commonly agreed data policy for users to best acknowledge the original data producers (e.g. by offering co-authorship and perhaps assignment of digital object identifiers for individual data sets). Obviously, a practical description of methods used, calibration etc. (so-called metadata) will also be included. This crucial first objective does not, in itself, require costly traveling to workshops. In essence the members are committed to send their datafiles to the common data centre, and advise their colleagues in any given experiment to do the same. Finally an official data publication or publication(s) will be realized in a suitable venue, for example an article in the special issue overall product of the WG (see item 4. below) and in *Eos* (Transactions Am.Geophys.Union). The database and experiences gained will provide an example for future next-generation *in situ* experiments.

2. Organization of 2-3 workshops where simulation modelers and key scientists of the experiments will meet. These workshops will be publicized in advance (SCOR website, other websites and newsletters) to
allow colleagues beyond the actual WG membership to express interest in participation. This may serve as a mechanism to involve additional colleagues from developing nations.

3. Organization of 2-3 special sessions of presentations at international marine science conferences, to encourage presentations from colleagues not yet involved in the activity.

4. Final publication of a suite of simulation modeling articles, as well as the common database (i.e. its brief description), and new synthesis papers based on data comparison, in a special issue of an oceanographic journal, as well as a multi-authored paper with recommendations for the next generation of in situ experiments.

Optional. Beyond the above 4 terms of reference to be accomplished, the WG may finally organize a training and education activity, for example, a summer school.

Data Management

The EUR-OCEANS Network of Excellence comprises a Data Integration and Networked Database task force with major objectives: (1) to rescue relevant historical datasets, (2) to organise long-term archiving of scientific information, (3) to develop an electronic portal for online access and dissemination. Dr. Nicolas Dittert as head of this task force will also be Full Member of the proposed SCOR WG, and relies on the permanent data centres World Data Centre-MARE (Bremen) and PANGAEA (AWI, Bremerhaven) for implementation of above Terms of Reference number 1. The WDC-MARE is within the WDC Network linked with the relevant data centres in North America (e.g. CDIAC at Oak Ridge), Asia and other regions. The World Data Centres will also ensure long term data storage.

Working Group Membership

Full membership and associate membership will aim for a good mix of junior and senior scientists in both categories, where senior colleagues are urged to pursue own funds for workshop participation, thus allowing optimal allocation of the WG budget to participation of junior scientists.

Membership will include a mixture of pivotal leaders of the various experiments, as well as various disciplines, as well as various modelers. In accordance with SCOR experiences, the Working Group will consist of 10 Full Members, no more and no less, among which two Co-chairs and 8 regular Members. These will be accompanied by a quite extensive group of Associate Members in order to ensure the necessary additional excellent expertise as well as involvement in the various in situ experiments, natural experiments, and simulation modeling. Both for Full Members and Associate Members, appropriate representation of both gender and developing country scientists will be achieved. Several more excellent scientists are envisioned to contribute datasets and/or modeling expertise via liaison with the Full and Associate Members, and workshops will be open to permit involvement of others. As a result of enthusiastic responses so far, please find below a suite of names of Liaison Scientists where more names will be added in due course.

<table>
<thead>
<tr>
<th>Name</th>
<th>Major Relevant Expertise</th>
<th>Experiment(s)</th>
<th>Nation</th>
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<tbody>
<tr>
<td><strong>Co-chairs:</strong></td>
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<tr>
<td>Lancelot, Christiane</td>
<td>prof. plankton ecosystem modeling</td>
<td>SOIREE</td>
<td>Belgium</td>
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<tr>
<td>Boyd, Philip</td>
<td>dr. plankton ecology</td>
<td>SOIREE, SERIES</td>
<td>New Zealand</td>
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<tr>
<td><strong>Full Members:</strong></td>
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<tr>
<td>Bakker, Dorothee</td>
<td>dr. CO2 system</td>
<td>S.O.JGOFS, SOIREE, EisenEx, CROZEX</td>
<td>UK</td>
</tr>
<tr>
<td>Bathmann, Uli</td>
<td>prof. polar mesozooplankton</td>
<td>S.O.JGOFS, EisenEx, Eifex</td>
<td>Germany</td>
</tr>
<tr>
<td>Coale, Kenneth</td>
<td>dr. iron-biota experiments</td>
<td>Ironex-1&amp;2, SOfEx</td>
<td>USA</td>
</tr>
<tr>
<td>De Baar, Hein</td>
<td>prof. iron and CO2, Geotraces</td>
<td>S.O.JGOFS, EisenEx</td>
<td>Netherlands</td>
</tr>
<tr>
<td>Dittert, Nicolas</td>
<td>dr. data management EUR-OCEANS and WDC-MARE</td>
<td>European Union</td>
<td></td>
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<tr>
<td>Minhan Dai</td>
<td>dr. ocean cycling of carbon and metals, Geotraces</td>
<td>China</td>
<td></td>
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<tr>
<td>Levasseur, Maurice</td>
<td>prof. DMS(P) and plankton</td>
<td>SEEDS-2, SERIES</td>
<td>Canada</td>
</tr>
<tr>
<td>Takeda, Shigenobu</td>
<td>prof. iron chemistry &amp; biology</td>
<td>SEEDS-1&amp;2, SERIES</td>
<td>Japan</td>
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<tr>
<td><strong>Associate Members:</strong></td>
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<tr>
<td>Assmy, Philip</td>
<td>dr. diatom responses</td>
<td>EisenEx, Eifex</td>
<td>Germany</td>
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</table>
SCOR WG Proposal: Legacy of in situ Iron Enrichments: Data Compilation and Modeling

Blain, Stephane prof. iron biogeochemistry KEOPS France
Buesseler, Ken dr. export production IronEx, SOFeX USA
Crook, Peter dr. iron chemistry Eisenex, SOFeX, Eifex Germany
Denman, Ken prof. modeling SERIES Canada
Goldson, Laura dr. tracer dispersion & mixing EisenEx, SOFeX UK
Follows, Mick dr. various modeling including OBCM's USA
Fujii, Masahiko dr. simulation modeling SEEDS-1&2, SERIES Japan
Hong, Huasheng prof. ocean biogeochemistry China
Kozyr, Alex dr. ocean CO₂ data management at CDIAC, Oak Ridge USA
Law, Cliff dr. tracer dispersion & mixing SOIREE, SERIES New Zealand
Marchetti, Adrian dr. diatom responses SERIES Canada
Mayer Branco, Pedro PhD plankton ecosystem modeling Eisenex Portugal
Nishioka, Jun dr. iron physical chemistry EisenEx, SEEDS-1&2, SERIES Japan
Rijkenberg, Micha dr. iron photoredox chemistry SOIREE, EisenEx UK
RutgersVanDerLoeff, Michiel, dr. export production/Geotraces S.O.JGOFS, EisenEx Germany
Schoemehl, Veronique dr. iron-phytoplankton, Phaeocystis Belgium
Strass, Volker dr. polar physical oceanography EisenEx, Eifex Germany
Tsuda, Atsushi prof. zooplankton ecology SEEDS-1&2, SERIES Japan
Tung, Yuan-Ho prof. marine chemistry and ecology Taiwan
Turner, Sue dr. DMS(P) cycles IronEx,SOIREE,EisenEx UK
Timmermans, Klaas dr. iron-diatom interactions EisenEx, KEOPS The Netherlands
Twining, Benjamin prof. intracellular iron SOFeX USA
Watson, Andy prof. CO₂ system, tracer dispersion SOIREE, EisenEx UK
Wingenter, O. prof. rarely studied trace gases SOFeX USA
Wang, Wen-Xiong prof. trace elements uptake and transfer in phyto-zooplankton China
Zhong, Shaojun dr. Geotraces Standards and Intercalibration task team China

Liaison Scientist:
(Liaison Scientists will be informed about and invited in all activities, they will submit datasets and/or are involved as simulation modeling experts. The below names merely are the beginning of a growing list of enthusiastic colleagues, each with excellent scientific credentials)
Gnanadesikan, Anand dr. ocean modeling including OBCM's, iron cycle USA
Le Clainche, Yvonnick dr. ecosystem DMS(P) modeling SERIES Canada
Nightingale, Philip dr. tracer dispersion, air/sea IronEx, EisenEx UK
Rivkin, Richard prof. bacterial responses SERIES Canada
Sanders, Richard dr. carbon export CROZEX UK
Sarmiento, Jorge prof. ocean modeling including OBCM's, iron cycle USA
Savoye, Nicolas dr. export production Eifex France
Vezina, Alain dr. ecosystem inverse modeling, DMS(P) Canada

Co-sponsorship(s) and Financial Support and Budget

The endorsement by international agencies SCOR, SCAR, SCOR-IGBP-SOLAS, SCOR-IGBP-IMBER, SCOR-GEOTRACES is deemed of primary importance for fostering the constructive, collaborative spirit essential to meet the terms of reference. The SOLAS SSC in its annual meeting, Amsterdam, May 2006, has fully endorsed this WG initiative. Similarly the IMBER SSC has been most positive at its annual meeting, Brest, May 2006. The proposal is also supported with great enthusiasm by the two co-chairs dr. Bob Anderson and prof. Gideon Henderson of GEOTRACES and will be listed on the agenda of the next GEOTRACES SSC to be held at end of year 2006.

Nevertheless SCOR is envisioned to take primary responsibility and accountability for the working group. Co-sponsoring by SCOR and SCAR jointly is envisioned. Informally the SCAR leadership and international office has been very positive thus far. This proposal is submitted to the Joint SCAR/SCOR Expert Group in Oceanography for its advice and endorsement at its second meeting at 10-11 July 2006 at Hobart, Australia.
This endorsement would support the submitted request to SCAR for co-sponsorship, to be discussed and decided at the XXIX SCAR Delegates Meeting, 17-19 July 2006 at Hobart, Australia.

The proposed co-chairs and full members now also are making efforts to realize significant if not major co-sponsorship by other agencies. Briefly the EUROCEANS Network of Excellence of the European Union has, in keeping with its major mission, agreed in principle to consider co-sponsorship for support of workshops as well as data management tasks. In practice the current proposal has been submitted to EUROCEANS for their existing schemes of subsidizing workshops and data management respectively. Similarly, the US NSF has been approached for support. Finally, the scientists among above membership from leading nations of iron enrichment experiments, notably Canada, New Zealand, Japan, Germany, United Kingdom, will be asked to pursue some support of their respective national agencies. Last, but not least, the above scientists of smaller nations, including Belgium and The Netherlands, will be asked for a similar effort.

The standard budget for a SCOR WG would allow organization of 3 workshops for 10-12 Full Members at a cost of US $ 15000 per workshop, i.e. in the order of US $ 45000 in total. The various above initiatives most likely would allow realization of this budget. Additional finances may well be realized towards supporting Associate members, as well as financing other costs such as data management expenses or publication costs.

References of overview articles each containing many more references


