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Acronyms

AD	Applicable document
ADB	Actions database
ADS	Analysis Dataset
AMOC	Atlantic Meridional Overturning Circulation
ATBD	Algorithm theoretical basis documents
BEC	Barcelona Expert Center
CCD	Closure Contract Documentation
CCI	ESA Climate Change Initiative
CDOM	Colored Dissolved Organic Matter
CDR	Climate Data Record
CMEMS	Copernicus Marine Environment Monitoring Service
CliC	Climate and Cryosphere
CSIC	Consejo Superior de Investigaciones Científicas
DIR	Directory
DNB	Debiased Non-Bayesian
DS	Dataset availability
DUM	Dataset user manual
DVP	Development and validation plan
EC	European Commission
ECMWF	European Centre for Medium-Range Weather Forecasts
EDS	Experimental dataset
EMI	Electromagnetic Interference
EO	Earth Observation
EOEP	Earth Observation Envelope Program
ESA	European Space Agency
ESL	Expert Support Laboratory
FMI	Finnish Meteorological Institute
FR	Final review
FWF	Freshwater fluxes
GCOS	Global Climate Observing System
GNSS	Global Navigation Satellite System
IAR	Impact assessment report
IASC	International Arctic Science Committee
ICES	International Council for the Exploration of the Sea
ICM	Institute of Marine Sciences
IEEC	Institut d'Estudis Espacials de Catalunya
IPCC	Intergovernmental Panel on Climate Change
ISC	Ice-Sea Contamination
ITT	Invitation to tender
KO	Kick-off
L2OS	Level 2 Ocean Salinity
LSC	Land-Sea Contamination
MFF	Multifractal Fusion
MR	Monthly report
MTR	Mid-term review
MTS	MIRAS Testing Software
MV-TN	Modelling and validation technical note
NS	Nodal sampling

PAR	Preliminary analysis report
PGICs	Peripheral glaciers and ice caps
PM	Progress meeting
PMP	Project Management Plan
PSU	Practical Salinity Unit
PVR	Product Validation Report
RB	Requirements baseline
RD	Reference document
RFI	Radio Frequency Interference
SAR	Synthetic Aperture Radar
SIAR	Scientific and impact assessment report
SMAP	Soil Moisture Active and Passive
SMOS	Soil Moisture and Ocean Salinity
SoW	Statement of work
SR	Scientific roadmap
SSS	Sea Surface Salinity
SST	Sea Surface Temperature
TDP	Technical data package
TN	Technical note
TPM	Third Party Missions
UPC	Universitat Politècnica de Catalunya
VIR	Validation and intercomparison report
VR	Validation report
WCRP	World Climate Research Programme
WP	Work package
WS	Workshop minutes
WWRP	World Weather Research Programme

1 Introduction

1.1 Scope of this document

This document holds the Science Roadmap (ScRM) prepared by Artic+ Salinity team, as part of the activities included in the [WP600] of the Proposal (Task 5 from SoW ref. EOP-SDR/SOW/084-17/DFP).

The objective of this document is to define a Scientific Roadmap for fostering future developments aimed at transferring the outcomes of the Arctic+ Salinity project into future scientific activities.

1.2 Structure of the document

The ScRM is structured as follows:

Chapter 1 describes the objectives of the documents.

Chapter 2 includes a detailed review of the interactions with Scientific community done in the context of this project. It also includes the presented proposals for projects in which we plan to use the project data generated on this project and the plans for papers publishing.

Chapter 3 performs a critical review of the products, and proposes some ideas for possible improvement of the product.

Chapter 4 show some of the Scientific studies which could be advanced thanks to the Arctic+SSS product. Those studies are divided between ongoing studies and future studies.

Chapter 6 contains the product assimilation plan into Copernicus Ocean Models.

Chapter 7 resumes the data distribution plan and presents two additional products which could be distributed based on ARCTIC+ SSS data

Chapter 8 describes the catch up and reprocessing plans.

Chapter 9 is the Summary and Conclusions section.

1.3 Applicable documents

ATBD	Algorithm Theoretical Baseline Document	Arctic+SSS-D3.1-ATBD_v1.0
DUM	Data User Manual	Arctic+SSS_DUM_D1.1_v1r2
RBD	Research Baseline Document	Arctic+SSS_RBD_D1.2_v1r6
SoW	Statement of Work	ref. EOP-SDR/SOW/084-17/DFP
PVR	Product Validation Report	Arctic+Salinity_WP400_PVR_v2r1
IAR	Impact Assessment Report	Arctic+Salinity_WP500_IAR_v1.0

2 Arctic+ Salinity interaction with the science community

We present here a resume of the scientific forums and relevant teams/projects where the product has been presented during the project time frame.

The Arctic+ Salinity team has participated in many workshops and meetings to present the work being developed during the project.

The (Table 1) below lists the Workshops, dates, title of the presentation and if it was oral or poster. Through these participation in workshops, the team presented the evolution of the project to the scientific community. The first presentation was on January 2019.

Workshop	Place and date	Title of the presentation	Type
Atlantic from Space	Southampton, UK January 2019	Arctic and North Atlantic Sea Surface Salinity retrieval	Oral LINK
ESA Living Planet	Milan, May 2019	Arctic+ Salinity: Retrieving Sea Surface Salinity in a Challenging Environment	Poster
Ocean Predict symposium 2	Halifax (Canada), May 2019	Evaluation of Arctic Ocean surface salinities from SMOS and two reanalyses against in situ data	Oral
IGARSS	Yokohama (Japan), July 2019	Arctic Sea Surface Salinity retrieval from SMOS measures	Poster LINK
Salinity Science Seminar	Hamburg, September 2019	Satellite SSS and simulated SSS in the Arctic (NERSC)	Oral
CCI Salinity Science Seminar	Hamburg September 2019	Overview of the Arctic+ Salinity ITT (BEC)	Oral LINK
AGU	San Francisco, EEUU December 2019	Arctic salinity from space: Monitoring the freshwater system.	poster
Ocean Science Meeting	San Diego, EEUU February 2020	Continental and sea ice melting signature in Arctic sea surface salinity.	Oral
CLIVAR/CliC Northern Ocean Regional Panel, NORP	February 2020	A new SSS product based on SMOS.	Webinar

ISAR - CANCELLED	Japan, March 2020	Assessment of the correlation between river discharge and sea ice growing in Laptev Sea	poster
EGU	online April 2020	BEC: CMEMS session: The SSS assimilation results	Oral Link
International Symposium of Marine Science	Online July 2020	ICM: Assessment of the correlation between river discharge and sea ice growing in Laptev Sea.	Oral
EO4 Polar Science	October 2020	ICM: Assessment of the correlation between SMOS and Sea Surface Salinity, river discharge and Sea Ice Fraction in Latpev and Kara Seas	Poster
EO4Polar Science (BEC)	October 2020	Remote Sensing to better assess the Arctic Freshwater fluxes budget - knowledge gaps towards improvements in collaboration ARCFLUX team (Henriette Skourup)	Discussion session
EGU Session OS4.6 – The Copernicus Marine Service (CMEMS)	2021	Impacts of assimilating Arctic surface sea salinities from SMOS in a coupled ocean and sea ice reanalysis	Pico Oral

Table 1 List of workshops where the work has been presented.

The (Table 2) below resumes the contacts done by the team with other scientist and teams looking for a collaboration on the context of Arctic+Salinity project:

Contacts	Project leader	Impact on Arctic+	Meeting
Oliver Wurl U. Oldenburg	PI of PassMe	In-situ surface salinity data in the Arctic.	2019, ESA LPS + teleconf
Séverine Fournier, Tony Lee JPL	Ocean Melting Greenland	Asked for in-situ data for validation https://omg.jpl.nasa.gov/portal/	2019, Discussed in EGU meeting
Jorge Vazquez	PODAC	Asked for in-situ and SMAP data	2019, Meet in Barcelona
Nick Hughes	KEPLER	Assimilating SSS in the TOPAZ will have impact on Copernicus roadmap for polar regions	2019, BEC + NERSC are part of the project.
CCI, Jacqueline Boutin (LOCEAN) + NOC.	CCI Option	Not advanced	ESA LPS + teleconf
Simon Yueh - Wendy Tang	SMAP PI	Intercomparison with SMAP	Ocean Salinity Science meeting-Paris.
Richard Jones, Paul Van Der Linden - MetOffice / Dirk Notz	CMUG / Mpeg	Would like to have the output of our project for modelling validation purpose.	2019 by email
Eric Bayler	NOAA	He asked for the Arctic+ SSS maps of 3 days	2019, Discussed in OS meeting
Joshua K. Willis	JPL - Ocean Melting Greenland	Info on how the OMG data was acquired	2019 by mail
Thomas Lavergne	MetNo	interested on the SSS maps	2019, by email
Chelle L. Gentemann	Farallon Institute / Earth & Space Research	interested on the L2 SSS maps (SMOS and SMAP) for Saildrone validation.	2020 tweeter
Rafael Gonçalves-Araujo	DTU Aqua	Interested in collaborate with M. Umbert in the SSS/CDM study in the Arctic Rivers, has in-situ data and previous knowledge (PhD and postdoctoral) in the area	2020 EO4Polar
Markus Janout	AWI	In situ data at the Laptev Sea. Data to validate SSS in the region and also validate the trends. Interested in future collaboration	2020 EO4Polar
Roshin P. Raj	NERSC	ESA Dragon cooperation. Title: "Pacific modulation of the Sea level variability of the Beaufort Gyre System in the Arctic Ocean"	

Johnny Johannessen - NERSC	Arktalas Project	Not easy inclusion of the Arctic+Salinity on Arktalas Project, studies were already ongoing	
Ian Fenty, JPL, USA	NERSC	Scientific exploitation. Interested in Greenland Ice sheet melt signatures West of Greenland	2019 Bergen

Table 2 List of contacts done for collaboration, exchange data or for asking specific questions.

Bellow we indicate the list of projects (some accepted others wating for resolution) that will use the data produced in this project:

Future projects and proposals based on using the Arctic+ SSS data:

- **CRIceS, H2020-LC-CLA-2020-2** (**approved** will start in September 2021): The upper ocean halocline is a regulator of and impacted by processes at the ocean/sea-ice interface. So, the ARCTIC SSS products developed in this project will be used to be compared with the salinity output of the current models participating in CMIP6. (**ICM**)
- **ARCTIC-MON, proposal submitted to the Agencia Estatal de Investigación (AEI) - Spanish funding (waiting for resolution)**: We propose to produce Arctic ocean classification product departing from the Arctic+SSS product to better asses and compute the freshwater budget and fluxes. (**ICM (PI)**)
- **Advanced insights into the Beaufort Gyre freshwater system from Space (ABS). ESA AO/1-10461/20/I-NB, ESA POLAR SCIENCE CLUSTER ITT (waiting for resolution):** This project has the focus on understanding of the Beaufort Gyre freshwater system. This project builds on the knowledge and data obtained from 13 individual projects: 11 ESA projects (ArcFlux, Arctic+salinity, CryoTEMPO among others) and 2 EU/EC projects. It will use range of Earth Observation (EO) data from satellites (Arctic+salinity product), in-situ and ocean & atmospheric reanalysis data during the Cryosat-2 era (2011-present). (**NERSC (PI) and ICM**)
- **Southern Ocean Freshwater (SO Fresh), ESA AO/1-10461/20/I-NB, ESA POLAR SCIENCE CLUSTER ITT (waiting for resolution):** Has the objective to derive sea surface salinity product from the Souther Ocean in collaboration with Southampton University. It will benefit of knowledge gained thanks to Arctic+ salinity, and also some software will be re-used. (**ARGANS (PI) and ICM)**
- **Pacific modulation of the Sea level variability of the Beaufort Gyre System in the Arctic Ocean**, ESA Dragon cooperation (**approved**). The sea level variability of the Beaufort Gyre (BG) is influenced by the changes in steric height and ocean mass. Hence the freshwater and heat stored in the BG can have significant impact on the sea surface height. Arctic+ SSS data will be used to study any link between sea surface salinity and freshwater content of the region estimated from available in-situ observations. (**NERSC (PI)**).

Planned papers:

- Paper with the **presentation of the product and its validation (started)**. This will be sent to the Earth Science System Data Journal (https://essd.copernicus.org/), which is a journal especially dedicated to the publication of articles on original research datasets, furthering the reuse of high-quality data of benefit to Earth system sciences. (BEC)
- Paper with applications when using the Arctic+ SSS product. This will contain the analysis of correlation between SSS and CDM in the Russian Arctic river discharge area. Latter, the relation has been used to derive SSS from CDM data, so we produce SSS maps of the region since year 2000. A correlation study with the river discharge will be done. Paper with the results of the assimilation of the Arctic+SSS product on TOPAZ. (NERSC)

3 Critical review of the Arctic+ Salinity product and further developments to advance

The description of the algorithm used to produce the product are reported in the ATBD, and the PVR summarize the validation and quality of the data. However, there is room for some improvements, already identified but which are out of scope of that project.

3.1 Better mitigation of the land/ice-sea contamination

The land/ice-sea contamination induces errors (mainly biases) on the retrieved SSS near the edge of the land and sea ice. The land/ice-sea contamination is mitigated in the current algorithm by subtracting the corresponding SMOS-based climatological value of brightness temperature to the measured value of brightness temperature, then adding back a good estimate of such climatological brightness temperature. This is the so-called debiasing method, that allows mitigation of systematic local biases at large extent. But the ice-sea contamination is not well corrected by this algorithm, since the edge of sea ice is not constant, and therefore a single SMOS-based climatology cannot correct the contamination effects. To ensure the minimum possible ice-sea contamination, all points having Sea Ice Concentration (SIC) > 0 according to the Sea Ice CCI product are discarded from the minimization process. The distance to the ice edge (defined by the line SIC=0) is also stored with the same purpose: minimize ice-sea contamination by avoiding the points too close to the ice in the L3 generation. Finally, to minimize ice-sea contamination and land-sea contamination all L2B points closer to 35 km to the ice edge or to the coastline are not considered in the L3 maps creation.

One possible method for correcting the land/ice-sea contamination that has not been applied in this version of the processor is the one described in the ATBD (section 2). This is to modify the correlation efficiency by means of a small percentage of change of the non-zero baseline elements of the Gkj matrix, as described in Corbella et al. (2015). However, in the last approved official reprocessing of SMOS L1, the adoption of Gkj correction was discarded because official L1 TBs are calibrated using NIR but Gkj correction works better with ALL-LICEF calibration; besides, as reported by Soil Moisture L2 teams, the quality of L2 Soil Moisture data was degraded when Gkj correction is introduced. Besides, the modification of Gkj is known to slightly increase the Ocean Target Transformation (OTT), what is also regarded as a degradation. Therefore, with the evidence available at this time the Gkj modification was discarded.

In the current L1/L2 across activities by SMOS Expert Support Laboratories, there is a dedicated task involving the computation and correction of the Point Spread Function (PSF) of SMOS antenna. It has been shown in Martínez et al. (2016) that SMOS antenna has a non-negligible PSF which induces long-range correlation errors and biases in the observed scenes; even more, the PSF was explicitly calculated from data acquired by the instrument. It is thought that the PSF is the likely origin of land/ice-sea contamination and even of the need for the OTT (that in that regard would be the sky-sea contamination). Correcting the PSF from SMOS data is a complicated task, because it is the same as making a deconvolution by the PSF kernel, what is an ill-posed mathematical problem. BEC is currently working on that correction, and they have managed so far to make a stable deconvolution of the scenes, although some unexpected large offsets appear – but the work goes on. It is expected that in a future, SMOS PSF will be corrected and then the land/ice-sea contamination will be removed altogether.

3.2 Better knowledge of the error on SSS associated to SST errors

It is well known that the sensitivity of L-band brightness temperature to SSS decreases as SST decreases. As a direct consequence, a given error in SST translates to a larger error in SSS at low SST than a higher SST (the error can be up to 4 times larger). It is then crucial to have an auxiliary SST field as accurate as possible, in order to minimize errors and biases. In Supply et al. (2020) they introduce an ad hoc correction on the CATDS SSS product which is directly derived from the standard L2 processor, in order to account for a different, better quality SST product (REMSS, which includes more satellites than the standard OSTIA/ECMWF); this leads to a significant improvement in quality of their product although the final quality indicators are not too good (when compared with in situ salinity, the standard deviation is 1.28 psu and the bias is 0.94 psu). The introduction of the debiased non-Bayesian approach (the one used in Arctic+ Salinity) allows to attain better scores, even if the SST product is not the best one, but it is clear that having a better SST will lead to significant improvement.

A recent result from another ESA project, Baltic+ Salinity, is that the behaviour of biases on SSS, and not only errors, is very different at the different values of SST. While the retrieval approach used in Baltic+ Salinity was a debiased non-Bayesian on SSS, while in Arctic+ Salinity is applied on brightness temperatures, the conclusions of their study on the propagation of SST errors is probably still pertinent for our project. In Baltic+ Salinity, the team discovered that it is necessary to include SST as an additional parameter for defining SMOS-based climatologies. That is, besides of separating the values in categories depending on longitude, latitude, xi, eta and overpass direction, they must also be separated depending on SST, because different SSTs lead to different biases and different errors due to the drastic changes with SST in the sensitivity of brightness temperatures to SSS. This also implies a change in which SMOS-based climatologies must be regarded, because with the inclusion of a new parameter the statistics at given conditions become so scarce that a different strategy must be adopted.

3.3 Improved climatology and more in situ data

A better SSS Arctic climatology with more in situ data would improve the product. This is a limitation for all the teams working with salinity data in the Arctic. For that, a large team of scientists from NASA, EEUU universities and other American institutions, led by Kyla Drushka, prepared a white paper with a project proposal to NASA, entitled “A NASA high latitude salinity Campaign” asking for financial support to developed a campaign to measure the SSS in the Arctic and Antarctic in different regions and periods. The proposal argue that those measurements could help to address several scientific questions such as: the near-surface Arctic stratification, Ice-edge dynamics, river runoff and Arctic freshwater balance and improvements in salinity remote sensing.

3.4 Advance on the algorithms to perform the debiasing non-Bayesian at SSS and avoid to use numerical models (HYCOM) on the corrections.

We hypothesize if performing the debiasing non-Bayesian method at SSS level and not at TB level could improve the final result. Based on work done in other semi-enclosed sea, we have noticed that the application of the debiasing at SSS level has resulted to be more effective (in terms of biases removing) than the debiasing in TB. Therefore, for future developments of the Arctic Ocean product, we propose to work with debiasing non-Bayesian at SSS level.

On the other hand, it is preferable not using any numerical model to perform the temporal correction of the data, to have a SMOS dataset independent to any model data source. Therefore, to perform the temporal correction we propose to compute global maps. Then, to compute the global mean from those maps and to impose that in time, the global mean is equal to the global mean of a constant salinity reference.

This temporal correction is only effective once the systematic biases (biases that are time independent) are previously removed (done with the debiasing non-Bayesian methodology).

Therefore, although from a theoretical point of view, the mitigation of systematic biases and the mitigation of temporal biases are independent, we expect having better performances after applying the debiasing at SSS level.

4 Additional scientific studies

Here we describe additional scientific studies that could be done to achieving the overarching scientific objectives of the project and the Arctic+ initiative. Some of them has been already started.

4.1 Ongoing work

- Assessing the impact of freshwater fluxes from the major Arctic rivers by exploiting the correlation between coloured detrital matter and Sea Surface Salinity.

The large freshwater river discharges entering the Arctic Ocean carry dissolved organic matter and suspended matter. Mixing of fresh river waters and saltier sea waters in the Siberian shelves forms large river plumes with a typical thickness of about 10 m. We are employing the improved SMOS Arctic+Salinity product together with standard optical CDM products (the colored dissolved and detrital organic materials absorption coefficient at 443 nm) to study the relationship between CDM and SSS. This represents a new potential for the study of the SSS/CDM relationship with a largely improved spatiotemporal monitoring compared to approaches that rely on in situ data in the area (Gonçalves-Araújo et al., 2015). The interannual and space co-variabilities of the SSS and CDM will be evaluated as this has important biogeochemical implications for marine biology and carbon cycle science. Notice that although SSS products have coarser resolution than CDM products, SSS is an all-weather product while CDM depends on cloud coverage and light conditions; therefore, SSS can be used to have reasonable operational estimates of CDM.

Assuming a conservative mixing relationship between both variables, we will explore the potential estimation of one variable using the other as a template, taking the advantage that the correlation between variables is high in the river plumes. This will allow us to go back in time and infer SSS estimations from CDM (data is available from the year 1998) to further assess the interannual variability of the river plumes and characterize the potential trends of freshwater entering the Arctic Ocean. Moreover, we intend to compute the surface area influenced by river water since 2012 and to estimate the volume of river freshwater using the mixed layer depth data from the TOPAZ model. The validation of these estimates will be done using river discharge data from Arctic Great Rivers Observatory and in situ measurements. We will check if one can observe changes on the river discharge volume, as stated in the literature.

It might be possible that some of the freshwater may be coming from local sea ice melting and not only from river discharge. However, during late summer and autumn, large river discharge determines the freshwater balance, while the contribution to sea ice melt is negligible (Osadchiev et al., 2021).

A possible follow-up study would consider vertical mixing, the dilution relationship and extrapolate CDM products where and when the optical data is not available for use in Arctic ecosystem models (assimilation/validation).

- Trends of Sea surface Salinity in the Arctic

We are working on analysing the SSS trends in the Arctic Ocean. For that work, we are using the enhanced SMOS SSS product generated through Arctic+Salinity, which spans 10 years. The analysis target six areas of special interest in the Arctic Ocean with special emphasis in the Beaufort Sea, where an increase in freshwater content is inferred from various in situ data as well as satellites altimeters (Proshutinsky et al. , 2019). The selected areas are: Norwegian Sea, South Norwegian Sea, Greenland Sea, Barents Sea, Beaufort Sea, Kara Sea and Laptev Sea.

The preliminary salinity trend analysis (reported in the Impact Assessment Report) shows promising results, even if the number of years analysed are limited due to RFI. The results obtained are coherent with the scientific publications on many regions: the freshening observed in the Beaufort Sea, the flat trend in the Barents Sea in the past decade, the freshening observed in Laptev Sea. However, more work is required on this line as well as to promote collaboration with other teams who have in situ campaign measurements to verify the results (Tarasenko et al. 2021).

- Greenland melting signal observed with SSS maps

First analyses show that some of the largest events of Greenland continental melting are observable with the SSS signal, but a deeper study should be performed. The first analysis was performed by J. Martinez and L. Bertino and it was presented in the Ocean Sciences Meeting 2020, San Diego, USA

(https://www.researchgate.net/publication/340966790_Continental_and_sea_ice_melting_signature_in_Arctic_sea_surface_salinity)

The study analysed the time lag that fresh water stays on surface before mixing it with other waters, and studies if eddies are visible in the surface due to the ice melting, etc.

4.2 Future Work

- Study the ocean dynamics combining SSS and SST

The Arctic Ocean has a strong density stratification that remains stable, because the effect of salinity on density is larger than that of temperature in that region. The freshwater coming from rivers and sea ice melting tends to stay at the surface due to its high buoyancy. Owing to the changes in the Arctic during the last years, in the absence of strong enough wind-driven stirring and with larger contribution of freshwater from rivers, stratification is increasing, strongly influencing water circulation in the Arctic ocean, sea ice formation, etc. We propose to use Arctic+ SSS, combined with other remote sensing data, to study ocean dynamics in Arctic Seas.

We will analyze six sea areas of special interest in the Arctic Ocean: Nordic Seas, Beaufort, Chukchi, East Siberian, Laptev, and Kara. Surface Quasi Geostrophic approaches allow to retrieve the streamfunction from surface buoyancy (derived from density, which in the Arctic is dominated by SSS). We will apply two SQG approaches (Isern et al., 2008; Wang et al., 2013) to reconstruct the ocean circulation (surface currents and vertical density anomalies) from satellite SSS and SST. We will intercompare these estimates with altimetry-based operational products (Globcurrent and OSCAR), and validate them using TOPAZ model reanalysis, in-situ measurements of surface drifters, and Sentinel-3 SLSTR and OLCI data to compare structure location of fronts and eddies.

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- <u>Freshwater lenses observed after melting</u>

First analysis of the SSS Arctic+ product show that in some occasions, we observe some freshwater lenses due to the melting.

Figure 1 is centred in September 16th. The figure shows a comparison of a 9-day average of daily OSISAF Sea ice concentration products and 9-day composite of SMOS SSS. One can observe spots with low concentration of sea ice, that coincide with freshwater spots in SMOS SSS. Note that SMOS composite is done taking into account 9-days, the retrieval at these spots is possible by merging some days affected by sea ice and others with the ice totally melted.

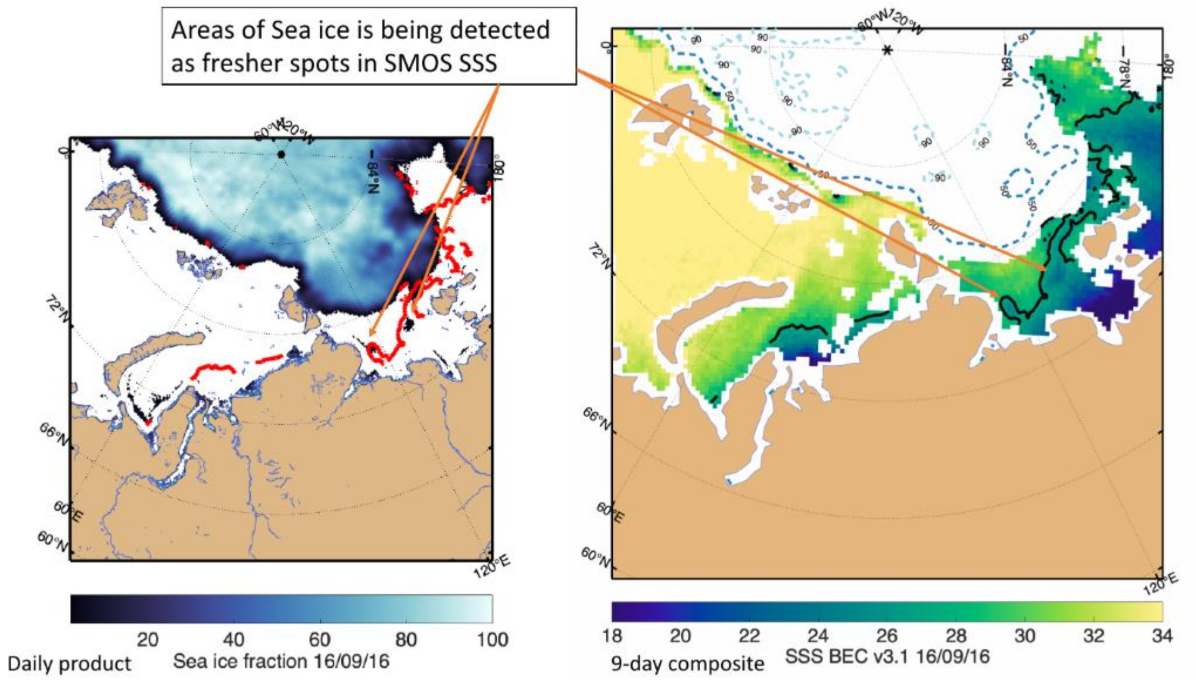

Figure 1 9-day averages daily Sea ice fraction product from OSISAF on Sep. 16 (left) and SSS v3.1 for the 9-day composite from the Sep. 16 (right). One can observe freshwater lenses in the arrows.

A more detailed exploration of the process can be seen in (Figure 2). Three-day composites of SMOS SSS for Sep. 11th-13th (top left) and Sep. 15th-17th (top right) compares with daily images of Sea ice concentration for September 7th, 10th, 12th and 16th (bottom row). Sea ice present in Sept. 7th totally disappears from 13th and the melted ice is seen as a fresh signature in 3-day SSS maps.

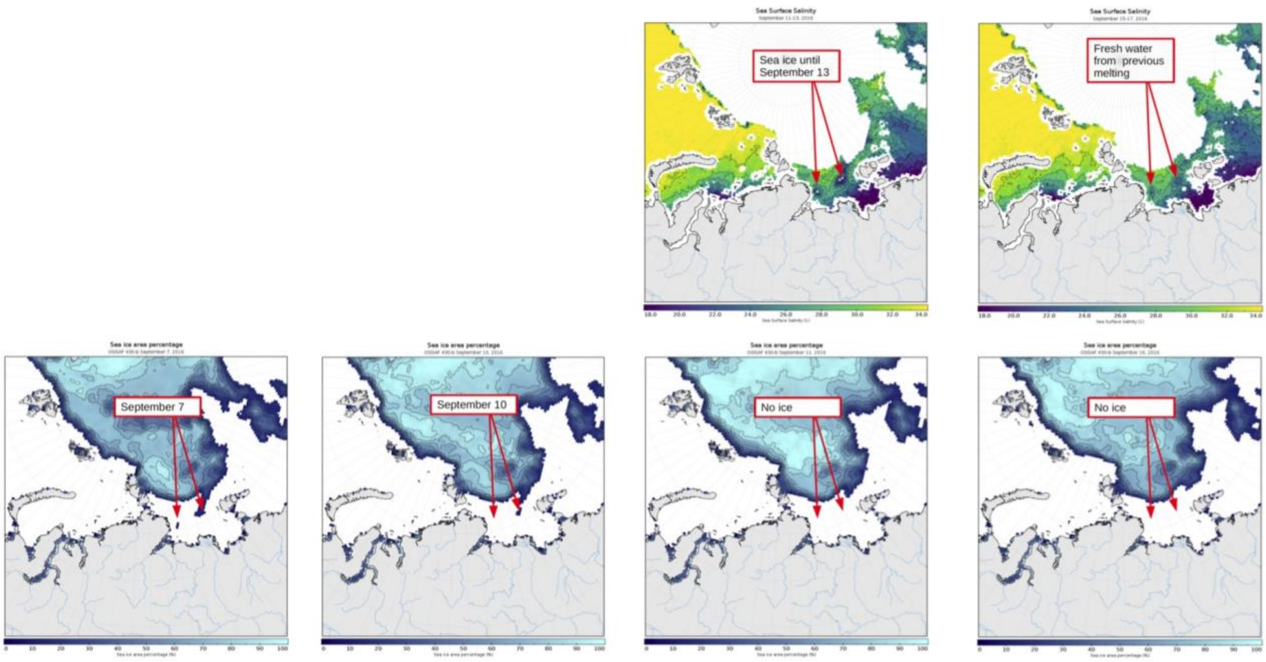

Figure 2 Three-day composites of SMOS SSS for Sep. 11th-13th (top left) and Sep. 15th-17th (top right) compares with daily images of Sea ice concentration for September 7th, 10th, 12th and 16th (bottom row).

- <u>Study of Freshwater fluxes / budget in the Beaufort Sea combined with SSH</u>

It should be feasible to study the freshwater system of the largest freshwater reservoir in the Arctic Ocean, the Beaufort Gyre, by using the SSS product produced under this project. The liquid freshwater content (in meters) (FWCL) could be computed following the equation described in Proshutinsky et al. (2009):

$$\mathrm{FWCL} = \int_{z2}^{z1} \frac{[Sref - S(z)]}{Sref} dz,$$

Therefore, the liquid freshwater content in the ocean surface could be estimating by using the Arctic+ SSS v3 product. This could be compared, with the freshwater content estimated using CryoSat-2 sea ice thickness products from the Alfred Wegener Institute (AWI) and the Centre for Polar Observation & Modelling (CPOM).

5 Arctic+ Salinity product assimilation plan into Copernicus ocean models

This section will focus primarily on the plans for the Copernicus Marine Services (CMEMS) with which NERSC is familiar. The Copernicus Climate Change Services (C3S) are also relevant for the uptake of the Arctic+ Salinity product and will briefly be mentioned below due to our lack of knowledge of the evolution of C3S in Copernicus 2. The CMEMS data assimilative ocean modelling products covering the Arctic are divided into Near Real Time (NRT) forecasts and analyses and long-term (20-30 years) reanalyses. The NRT forecasts products are the following:

- The TOPAZ4 analyses and forecasts produced by MET Norway for the Arctic Monitoring and Forecasting Center (ARC MFC), led by NERSC.
- The analyses and forecasts produced by Mercator Ocean International (MOi) for the Global MFC.
- The coupled analyses and forecasts produced by the UK MetOffice for the Global Coupled MFC.

The reanalysis products are the following:

- The TOPAZ4 reanalysis managed by NERSC for the Arctic Monitoring and Forecasting Center (ARC MFC)
- The GLORYS 1/12 reanalysis managed by Mercator Ocean International for the Global MFC.
- The Global Reanalysis Ensemble Product (GREP) merging four reanalysis products from UK Metoffice, CMCC, MOi and ECMWF. The ECMWF "member" of GREP is also distributed through C3S.

All of these products are using data assimilation and have the technical capability and expertise to assimilate SSS from space. All MFCs have to comply to the CMEMS continuous upgrade calendar by submitting Requests for Change documenting the improved quality of the service three months before the scheduled Entry Into Service (EIS). The EIS are generally occurring three times a year in March, July and December, except in the transition year 2021 when only two EIS are scheduled in May and December 2021. The CMEMS MFCs must give priority to the assimilation of CMEMS data sources and Global MFCs give priority to the assimilation of global datasets rather than regional datasets. In this landscape the nearest entry point of the Arctic+Salinity SSS product is the assimilation into the Arctic MFC reanalysis.

Several C3S data assimilative systems provide seasonal to interannual forecasts (among which the ECMWF, CMCC, UK MetOffice, Meteo France and NCEP) also tend to favour the global observations for identical reasons as the CMEMS global systems, to avoid discontinuities at the boundaries of the Arctic domain.

A direct provision of the Arctic+Salinity SSS data, as every ECV, falls within the scope of the C3S and CMEMS services, but the present organisation of contracts under each service does not leave room for the inclusion of a regional Arctic SSS product (CMEMS has thematic assembly centres for SST, sea level, sea ice, ocean colour, winds, waves and a global multi-observations center, but the SSS does not fall within the realm of any of them). MOi has the issue well in mind and will make space for Arctic SSS products within Copernicus 2 (PY le Traon, pers. comm.). The standard conditions are the validation of SSS products against in situ salinity measurements (particularly those hosted by CMEMS), adhering to CMEMS standard NetCDF4 format and metadata and regular updates of the time series at least twice a year. A near-real-time processing of SMOS SSS would be desirable for assimilation in CMEMS ocean forecasts but not strictly required since multi-year products have a value on their own.

One complication as of Copernicus-1 is that CMEMS and C3S have no mechanism to coordinate their data products, which can lead to inconsistencies between their catalogues of ECVs. CMEMS and C3S are presently investigating the possibility of joint procurements for the second phase of Copernicus, for which the Arctic SSS product would be a legitimate candidate.

The Arctic MFC is presently producing an upgraded TOPAZ4b reanalysis with double vertical resolution. At the time of writing this report, the years 1991-2013 are already provided through CMEMS in the product ARCTIC_MULTIYEAR_PHY_002_003 and NERSC plans to add the period 2014-2020 on 14th December 2021. Since the Arctic+ SSS product is now approved for distribution, the plan is to assimilate the SSS data in the ongoing TOPAZ4b reanalysis from 2013 onwards, discarding 2011 and 2012 in order to avoid most of the RFI contaminations.

The Copernicus 2 services contracts are expected to be re-opened for competition in the Summer 2021 and the first release of the Copernicus 2 CMEMS should enter into service in 2022.

6 Arctic+ Salinity data distribution

Arctic+ Salinity and BEC webpage

The product will be freely distributed in the web page of the project, held in ARGANS website (https://arcticsalinity.argans.co.uk) and through the BEC server webpage (http://bec.icm.csic.es/) in netCDF format.

The data is published here https://digital.csic.es/handle/10261/219679?mode=full and the data has the following DOI 10.20350/digitalCSIC/12620.

COPERNICUS / CMEMS

The distribution of the Arctic+ product to Copernicus has been discussed with Pierre Yves Le Traon through Laurent Bertino (see Section 6 above). Le Traon commented (in a personal communication) that this issue is under discussion for new phase Copernicus 2 from 2022. It seems that two SMOS salinity datasets (SSS CATDS and BEC products) could be distributed though CMEMS. It is not clear yet, in which TAC it would fit.

EMODNET

EMODnet is a long-term marine data initiative supported by EC DG MARE. It has been developed through a step-wise approach and is currently in its third and final development phase. Available data are used to create and make available multi-resolution maps of all Europe's seas and oceans, spanning all seven disciplinary themes (physics, bathymetry, geology, sea bed habitats, chemistry, biology, human activities). More than 120 partner organisations are currently involved in the EMODnet programme; new contributors are always welcome via the EMODnet Associated Partnership Scheme.

PANGAEA

The information system PANGAEA is operated as an Open Access library aimed at archiving, publishing and distributing georeferenced data from earth system research. The system guarantees long-term availability of its content through a commitment of the hosting institutions.

Most of the data are freely available and can be used under the terms of the license mentioned on the data set description. The description of each data set is always visible and includes the principal investigator (PI) and the project who may be asked for access.

Each dataset can be identified, shared, published and cited by using a Digital Object Identifier. PANGAEA also allows data to be published as supplements to science articles or as citable data collections in combination with data journals like ESSD, Geoscience Data Journal, Scientific Data, or others.

The PANGAEA data editorial ensures the integrity and authenticity as well as a high usability of your data.

Centro Nacional de Datos Polares

The National Polar Data Center (CNDP) comprises the Spanish Polar Archive (http://hielo.igme.es/index.php/es/). This is an initiative of the Spanish Polar Committee (CPE) whose Technical Secretariat is in charge of coordinating all the activities corresponding to the National Antarctic Authority.

The CNDP is now coordinated by the UTM division- Institut de Ciències del Mar of Spain (ICM). Among its tasks are the administration of the metadata generated by Spanish investigations in the Polar field and the storage, management and dissemination of documentary collections, all under the supervision of the CPE.

PIMEP

Under this project, and thanks to the extensive validation we have done during the project, we have realized that the standard validations done in PIMEP does not reflect the validity and quality of this product. Specially, because the standard validation (mean, median, std, RMSE, etc.) does take into account the improved spatial resolution. The team considers that other mathematical tools should be used for the validation process of a product, as for example the Spectral Analysis, and the Triple collocation, as explained in the PVR of this project. So we encourage the PIMEP coordinators to add those validation methodologies. However, at the moment the Arctic+ V3.1 product is being served and analysed in the PIMER webpage.

Additional products based on ARCTIC+ SSS DATA

- Generate and distribute daily TB maps

The improved TB maps produced under this project will be very valuable to produce other polar geophysical variables products. For example, the generated TB, called 1C, data could be used to derive Sea Ice Thickness (SIT) and Sea Ice Concentration (SIC) data from SMOS. That product, L1c, is TB per orbit, at Top of the Atmosphere (TOA) but with the Faraday correction done and the geomagnetic field corrected (see ATBD pg 19 for more information). That L1c is computed with the geoMTS software starting from the official ESA L1b product.

To derive SIT maps from SMOS TBs several algorithms are described in the literature (Kaleschke et al., 2012; Huntemann et al., 2014, Gupta et al., 2019). The method to derive sea ice concentration from SMOS TB, is described in Gabarro et al., 2017.

The assimilation of TB instead of processed SIC and SIT is also possible if the function TB (SIC,SIT) is used as an observation operator in the data assimilation system, similarly to the assimilation of radiances in operational weather models. OASYS (F. Kauker) and MET Norway (T. Lavergne) are strong proponents of this approach.

- Arctic sea surface water classification product

Specific global ice-free Arctic classification maps of water types using SMOS SSS product (from Arctic+ Salinity) and CDM data from satellite optical sensors during cloud-free days spanning the full 10-year SMOS lifetime could be generated. The new product would be useful to discriminate between different surface water types in the Arctic Ocean. SMOS observe regions influenced by large rivers and the seasonal ice edges, where freshwater from river discharges and sea ice melt both contribute to the salinity variability. We will separate low-salinity waters from rivers (RW) or from ice-melt (MW) as compared with seawater (SW). A first attempt was done in Matsuoka et al., (2016), but no specific product was distributed. The proper separation and classification of these types of water is needed to better understand physical and biogeochemical processes. These products will be useful to study the dynamics of several biogeochemical processes occurring in the Arctic Ocean such as algal blooms and their potential link with ice melting and nutrient supply. These products will also be useful to gain knowledge on the relation between atmospheric aerosols, sea salinity, and CDM.

7 Arctic+ Salinity data catch-up and re-processing plan

7.1 Catch up processing

We will produce the Arctic+ Salinity SSS v3.1 for 2020. For that, we need to update some auxiliary files in our BEC internal chain.

Every 6 months we would like to do a catch-up campaign to produce the Arctic SSS v3 products until the end of the mission, time-permitting.

7.2 Reprocessing

New L1B v724 is already in the BEC facilities. As part of the ESL activities, BEC internal chain is currently being updated to be able to read this new version of the L1B products (introduction of the artificial scene library). Once this is ready, we could then process the data up to SSS v3.1 maps using the algorithms and software defined under this project.

Every 6 month we would like to do a catch-up campaign to produce the new Arctic SSS v3.1 products until the end of the mission, if time permits.

8 Summary and Conclusions

The impact that represents the Arctic+ SSS project is huge in different directions:

First, we have developed a new dedicated SSS Arctic product released to Scientific community with better performance than the previously available products, especially for the improved spatial resolution (see Product Validation Report).

Moreover, it has been demonstrated the positive impact of its assimilation on TOPAZ, described in the Impact Assessment Report document. So, from now on, TOPAZ system will assimilate the Arctic+ SSS product. This will hopefully be set on the system in the next phase of Copernicus.

Arctic+ salinity product presented in this document may aid the Arctic Scientific community in promoting the current state of the art of different oceanographic challenges. The science applications of SSS in the Arctic will go beyond the science applications seen along the course of this project (see IAR). Therefore, SSS data produced within this project will be included in the Essential Climate Variables (ECV) inventory (v3.0) (ref. To ECMF ECV inventory website)

Several scientific studies based on the new product have been started and other ideas are proposed in this document which need further development.

Moreover, the new daily TB product used to derive the SSS product could be released to scientific community.

The team has gained knowledge on how to process SMOS TB measurements in cold waters regions. This knowledge will be useful for future developments to produce SSS in the Southern Ocean, for example.

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