



# Assimilation of sea surface salinities from SMOS in an Arctic coupled ocean and sea ice reanalysis

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1 **Abstract** 2 In the Arctic, the sea surface salinity (SSS) plays a key role in processes related to 3 water mixing and sea ice. However, the lack of salinity observations causes large 4 uncertainties in Arctic Ocean forecasts and reanalysis. Recently the Soil Moisture and Ocean 5 Salinity (SMOS) satellite mission was used by the Barcelona Expert Centre to propose an 6 Arctic SSS product. 7 In this study, we evaluate the impact of assimilating this data in a coupled ocean-ice data 8 assimilation system. Using the Ensemble Kalman filter from July to December 2016, two 9 assimilation runs assimilated two successive versions of the SMOS SSS product, on top of a 10 pre-existing reanalysis run. The runs were validated against independent in situ salinity 11 profiles in the Arctic. The results show that the biases and the Root Mean Squared 12 Differences (RMSD) of SSS are reduced by 10% to 50% depending on areas and put the 13 latest product to its advantage. The time series of Freshwater Content (FWC) further show 14 that its seasonal cycle can be adjusted by assimilation of the SSS products, which is 15 encouraging for its use in a long-time reanalysis to monitor the Arctic water cycle. 16 17 Keywords: Arctic Ocean; Sea Surface Salinity; FWC; SMOS;





### 1. Introduction

- 19 The Arctic Ocean is undergoing a dramatic warming, causing the loss of sea ice area
- 20 coverage visible on satellite data (Johannessen et al., 1999; Stroeve and Notz, 2018). The
- 21 sea ice melt contributes freshwater to the Arctic Ocean, together with other sources and has
- 22 far-reaching effects on the Arctic Ocean environment, as reviewed in Carmack et al. (2016).
- 23 A recent update of the review paper showed a stabilization of the Freshwater Content (FWC)
- 24 of the Arctic Basin, although observations indicate that the Beaufort Gyre keeps freshening
- 25 (Solomon et al., 2021). The Arctic observing system, contrary to other oceans, lacks the
- 26 capability to provide a complete picture of the ocean salinity, particularly because of
- 27 obstruction by sea ice.
- 28 A complete reconstruction of Arctic environmental variables requires a data assimilative
- 29 numerical model capable of propagating information below sea ice during the winter as
- 30 practiced by ocean operational forecast systems (Dombrowsky, 2009; Fujii et al., 2019). As
- 31 for other ocean data assimilation (DA) applications, the Arctic reanalysis products of ocean
- 32 and sea ice play an important role in understanding climate change and its mechanisms. In
- 33 recent years, many studies (Storto et al., 2019; Uotila et al., 2019) evaluated the quality of
- 34 the Arctic reanalysis products and recommended experiments maximizing the usefulness of
- 35 new available observations, such as done in Kaminski et al. (2015) or Xie et al. (2018)
- 36 among others. However, there are no impact studies of salinity observations in the Arctic to
- 37 our knowledge.
- 38 Ocean salinity has been used to study the water cycle for the last 20 years (e.g., Curry et al.,
- 39 2003; Boyer et al., 2005; Yu, 2011; Yu et al., 2017). The salinity variations have far-reaching
- 40 implications for ocean mixing, water mass formation, and ocean general circulation, but still
- 41 suffer from large uncertainties, mainly due to sparse observations and the lack of a steady-
- 42 state reference time period (e.g., Stroh et al., 2015; Xie et al., 2019). Measuring sea surface
- 43 salinity (SSS) from passive microwave remote sensing is a comparatively new but promising
- 44 way to reduce the uncertainty in salinity. Launched in November 2009, the Microwave
- 45 Imaging Radiometer using Aperture Synthesis (MIRAS) instrument of the European Space
- 46 Agency's (ESA) Soil Moisture and Ocean Salinity (SMOS) mission measures the brightness
- 47 temperature (T<sub>B</sub>) on the sea surface. The passive 2-D interferometric radiometer on the
- 48 satellite operating in L-band (1.4 GHz) is sensitive to water salinity and sufficiently free from
- 49 electromagnetic interference (e.g., Font et al., 2010; Kerr et al., 2010). Since May 2010,
- 50 SMOS operationally provides SSS records over the global ocean (Mecklenburg et al., 2012).
- 51 Furthermore, the assimilation of satellite derived SSS products using an ensemble DA
- 52 method has been found to significantly improve the surface and subsurface salinity fields in
- 53 the tropics (Lu et al. 2016). The advantages of assimilating three SSS products from SMOS,
- 54 Aquarius (ref., Lee et al, 2012), and Soil Moisture Active Passive Mission (SMAP; e.g., Tang





- et al., 2017) into a global ocean forecast system using 3D-Var DA method have also been
- 56 demonstrated by Martin et al (2019). Their results show benefits of assimilating both the
- 57 SMOS and SMAP datasets in the intertropical convergence zone in the tropical Pacific.
- 58 However, there are very few studies to investigate the impacts of assimilating SSS products
- 59 in Arctic or high latitudes. There are three main reasons for this: i) the lower sensitivity of T<sub>B</sub>
- 60 in cold waters leading to larger SSS error (Yueh et al., 2001) (e.g, the sensitivity drops from
- 61 0.5 to 0.3 K PSU<sup>-1</sup> when the sea surface temperature decreases from 15 to 5°C); ii) Land-
- 62 sea and ice-sea contaminations resulting from the abrupt changes of of T<sub>B</sub> values across
- 63 these two interfaces, combined with the large ground footprint of SMOS; and iii) The removal
- 64 of biases ideally requires a well-observed steady-state period, from which climate change
- 65 has deprived us. Addressing these challenges in the SMOS salinity retrieval approach,
- 66 Olmedo et al. (2017) introduced a non-Bayesian retrieval method to debias the Level 1
- baseline (L1B) salinity against the reference SSS from Argo data.
- 68 Starting from ESA L1B (v620) product of T<sub>B</sub> from SMOS, the Barcelona Expert Centre (BEC)
- 69 released the version 2 Arctic gridded SSS product with a regular grid by 25 km resolution
- 70 (e.g., Olmedo et al., 2018) via their portal (http://bec.icm.csic.es/; last accessed March 2019).
- 71 The V2 SSS regional product was produced for the Arctic domain during the time-period
- 72 2011-2016. Xie et al. (2019) evaluated this earlier SSS product and found considerable
- 73 discrepancies among the six SSS products in the Arctic, especially in the freshest seawater
- 74 (<24 psu). The intercomparison of these Arctic SSS products shows room for improvement
- 75 of the SMOS-based SSS in the Arctic.
- 76 Recently, under the framework of the ESA project Arctic+Salinity and further developing the
- 77 non-Bayesian scheme, the effective resolutions were enhanced both in space and time. The
- 78 new version of SSS product (V3.1) shows advantages for monitoring the mesoscale
- 79 structures and the river discharges (e.g., Martínez et al., 2022), and was released through
- 80 the BEC portal (also at doi: 10.20350/digitalCSIC/12620; last accessed May 2022). It also
- 81 provides daily maps of 9-days averages in the Arctic on the regular 25 km grid and covers a
- 82 longer time-period 2011-2019. The major differences in the estimation of the two SSS
- 83 products (V2.0 and V3.1) are detailed in the Algorithm Theoretical Baseline Document
- 84 (ATBD) of the Arctic+Salinity project (Martínez et al., 2020). Another SMOS-based Arctic
- 85 surface salinity product from LOCEAN (Supply et al. 2020, Boutin et al., 2022) has been
- released posterior to Xie et al. (2019), but not assimilated in this study.
- 87 The two successive versions of the BEC SMOS SSS products are assimilated in the
- 88 TOPAZ4 Arctic reanalysis system during the summer 2016, and compared to the Arctic
- 89 reanalysis without assimilation of satellite SSS data, which consistes the Arctic reanalysis in
- 90 the Copernicus Marine Services at that time. The model validation against independent





91 observations will show the differences stemming from these two products, although they are

92 originating from the same initial data source (SMOS). Their effect once assimilated in an

93 Arctic coupled ice-ocean model shows large differences, thereby also motivating further

94 efforts to improve SSS retrievals in the cold Arctic.

95 The paper is organized as follows: Section 2 describes briefly the coupled ocean and sea ice

96 data assimilation system and the assimilation experiments; Section 3 describes the in situ

97 observations and the validation metrics; The results are presented in Section 4 which

98 includes the validation using independent SSS observations, separated into different ocean

99 basins. Section 4 also analyses the impact of the assimilation using the regional SSS

100 assimilation increments, and explores the integrated effect on the freshwater contents in the

101 model. In Section 5, the findings of this study and future perspectives are summarized.

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# 2. Assimilation system and experimental design

2.1 The Arctic ocean and sea-ice coupled data assimilation system

TOPAZ was built as a coupled ocean and sea ice data assimilation system, using the

ensemble Kalman filter method (EnKF; Evensen 2003) to assimilate consistently multiple

types of observations in the ocean and sea ice (Xie et al., 2017). The ocean model in this

108 system uses the version 2.2 of the Hybrid Coordinate Ocean Model (HYCOM; Chassignet et

109 al., 2003) with a low-distortion square grid of horizontal resolution of 12-16 km. The coupled

110 sea ice model uses a single category thermodynamic model (Drange and Simonsen, 1996)

111 combined with the dynamics of the modified elastic-viscous-plastic rheology (Bouillon et al.,

112 2013). The model covers the whole Arctic basin excluding the Pacific Ocean. A seasonal

inflow is imposed across Bering Strait, based on observed transports (Woodgate et al.,

114 2012). At all lateral boundaries, the temperature and salinity stratifications are relaxed to a

115 climatology combining the 2013 World Ocean Atlas (version 2.0 of WOA13; Zweng et al.,

116 2013) and the Polar science ceter Hydrographic Climatology version 3.0 (PHC; Steele et al.,

117 2001) with a 20-grid cells buffer zone. To avoid a potential model drift, the surface salinity is

118 relaxed to the same climatology with a 30-day timescale, and the relaxation is turned off

119 wherever the difference from climatology exceeds 0.5 psu. The salinity flux from the SSS

120 relaxation thus spreads evenly into the mixed layer depth without creating a new stable fresh

121 layer at the surface.

122 The TOPAZ model runs an ensemble of 100 members. On a weekly basis, the

123 Deterministic Ensemble Kalman Filter (DEnKF; Sakov et al., 2012) then assimilates different

124 types of ocean and ice observations, including along-track sea level anomaly (SLA), sea

125 surface temperature (SST), in situ profiles of temperature and salinity, sea ice concentrations

126 (SIC) and sea ice drift products all sourced from the Copernicus Marine Environment





Monitoring Services (CMEMS). The two steps of the assimilation system can be simply translated by the following expressions (update and model propagation):

$$X_a = X_f + K(y - HX_f) \tag{1}$$

$$X_f = M(X_a) \tag{2}$$

Where the matrix **X** represents the model states with all 3-D and 2-D variables needed by the model forward integration, represented by the operator **M**. The subscripts 'a' and 'f' respectively indicate the analyzed model state obtained through optimization after DA, and the model forecast. The vector y is composed of the quality-checked observations during the weekly cycle, the observation operator *H* gives the model equivalent matching the observations. The innovation term (in parenthesis in Eq.1) represents the differences between the model and the various observations on the observation space. The **K** matrix (Kalman gain), is calculated as in Sakov et al. (2012) and updated in Xie et al. (2017). The same TOPAZ4 system provides a 10-days' forecast of ocean physics and biogeochemistry in the Arctic everyday via the CMEMS portal.

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2.2 The assimilation experiments and the observation error estimate for SSS To evaluate the impact of the two versions of the SSS products, a control assimilation experiment (Exp0) and two parallel assimilation experiments (ExpV2, ExpV3) were performed in the time period from July to December 2016. Exp0 assimilates all available ocean and sea ice data, except the satellite SSS product. On the other hand, ExpV2 and ExpV3 additionally assimilate the BEC SSS product V2.0 and V3.1 respectively. The main differences of the three assimilation runs of ExpV2 and ExpV3 are detailed in Table 1. Since the salinity errors from Passive Microwaves are higher in high latitudes than elsewhere, the zonal average of standard errors north of 60°N were previously estimated around 0.6 psu (Vinogradova et al., 2014). Later on, the intercomparison of different SSS products including the climatology, satellite, and the Exp0 reanalysis showed that the discrepancies were a decreasing function of salinity (Xie et al., 2019). This relationship seems qualitatively reasonable as the spatio-temporal variability and representativity errors are often higher in areas of fresher water, but quantitatively they combine the errors of the remote sensing products, models and climatologies and may be larger than the remote sensing errors alone. Still, we use an error function for ExpV2 and ExpV3 adjusted to the discrepancies as shown in Eq. 3:

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$$\delta_{SSS} = \max \left\{ \delta_{int}, \left[ 0.6 + \frac{6}{1 + exp\left( \frac{SSS - 16}{5} \right)} \right]^2 \right\}$$
 (3)

Where  $\delta_{int}$  is the instrumental error variance estimated by the data provider. In ExpV2, it is set to zero due to their absence. Eq. 3 yields more conservative error estimates than the providers, which also reduce the inconsistencies caused by strong assimilation updates.





- 163 Other such precautions are applied following Sakov et al. (2012). By construction, the
- 164 observation errors are always larger for the V3.1 than the V2 product, but in fresh waters
- 165 they are identical. This implies that the assimilation may pull the analysis closer to the V2
- than the V3.1 product in the more saline waters but are otherwise treated on equal footing,
- ignoring that the more recent product is a priori expected to be more reliable.

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#### 3. In situ SSS observations for validation

- 170 All in situ salinity profiles were collected from various repositories and cruises (as shown in
- 171 Fig. 1). The salinity measurements were extracted near the surface over the Arctic domain
- 172 during the experimental time period and sanity-checked. Since the model does not reproduce
- 173 local gradients of the vertical salinity profiles shown in Supply et al. (2020), all the salinity
- 174 profiles are averaged over the upper 8 meters below the surface. This also avoids the loss of
- the profiles that do not reach the surface.
  - Data from the Beaufort Gyre Experiment Project (BGEP)
- 177 The BGEP has maintained an observing system in the Canadian Basin since 2003 and
- 178 provides in-situ observations over the Beaufort Gyre every summer. Although the BGEP has
- 179 maintained three bottom-tethered moorings since 2003, the shallowest depth of the
- 180 measured profiles for temperature and salinity is below 50 m. Hence, in this study, we only
- 181 use the Conductivity Temperature Depth (CTD) dataset from the cruise in 2016
- 182 (https://www2.whoi.edu/site/beaufortgyre/data/ctd-and-geochemistry/, last access: 14<sup>th</sup>
- February 2022). SSS observations from these CTD profiles in the time-period from 13<sup>th</sup> Sep
- to 10<sup>th</sup> Oct 2016 are represented by the red triangles in Fig.1.
- Data from Oceans Melting Greenland (OMG)
- 186 The project Oceans Melting Greenland was funded by NASA to understand the role of the
- 187 ocean in melting Greenland's glaciers. Over a five-year campaign, this project collected
- 188 temperature and salinity profiles by Airborne eXpendable Conductivity Temperature Depth
- 189 (AXCTD) launched from an aircraft (e.g., Fenty, et al, 2016). The deployed probe can sink to
- 190 a depth of 1000 meters, connected with a float by a wire. The measured temperature and
- 191 conductivity are then sent back to the aircraft. These salinity profiles collected during the first
- 192 OMG campaign in 2016, are downloaded from
- 193 https://podaac.jpl.nasa.gov/dataset/OMG L2 AXCTD/ (last access: 10th February 2022). The
- 194 SSS from OMG distributed around Greenland, from 13th Sep to 10th Oct 2016 are shown as
- the inverted red-triangles in Fig. 1.
- Data from the International Council for the Exploration of the Sea (ICES)
- 197 Salinity profiles were also obtained from the ICES portal (https://www.ices.dk). Shown as
- blue squares in Fig. 1, the locations of the profiles during the last 6 months of 2016 are



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dense in the Nordic Seas, and restricted to the north of 58°N for this study. Valid salinity profiles from ICES (last access: 9<sup>th</sup> February 2022), are obtained from 6<sup>th</sup> July to 23<sup>rd</sup> Nov in 2016

• Data from other cruises at the Arctic Data Center (ADC)

203 Surface salinity observations from scientific cruises are obtained from the Arctic Data 204 Center portal (https://arcticdata.io/catalog/data; last access: 17th Feb 2022). During the 205 model experiment, the first relevant cruise in ADC was SKQ201612S which was operated by 206 University of Alaska Fairbanks with the RV Sikuliag. This cruise collected data from Nome, 207 Alaska on 3rd September, to the northeast Chukchi Sea, and then back to Nome at the end of 208 September 2016. The temperature and salinity profiles were collected by a Sea-Bird 911 209 CTD instrument package. All measurements at each station were done both down- and up-210 cast ways. To produce water column profiles at each station, the down-cast data were 211 binned at 1 m intervals (Goñi et al., 2021). Besides the CTD profiles of SKQ201612S, more 212 seawater samples were collected via the surface underway system on the RV Sikuliaq. 213 Through a sea chest below the waterline (eg., 4-8 m), the uncontaminated seawater was 214 pumped into the ship and the corresponding filtration system supplies samples every 3 hours 215 to the sensors (More details in Goñi et al., 2019). These SSS observations were obtained 216 from 9th to 27th September, indicated as blue crosses in Fig. 1. 217 Moreover, SSS measurements were also collected from the Seabird CTD on board Sir 218 Wilfrid Laurier (SWL) vessel but only in July 2016. This cruise is part of the annual monitoring 219 from the Canadian Coast Guard Service (Cooper et al., 2019). The SSS observations are 220 obtained near the Bering Strait close to the Pacific boundary of our model. 221 After removing the effect of diurnal cycle in observed surface salinity, all valid SSS 222 measurements from the above data sources are compared with the daily average SSS of the 223 three assimilation experiments listed in Table 1. All the assimilation runs use a weekly 224 assimilation cycle: the model runs forward 7 days after each assimilation step and provides 225 daily averages for each day from the ensemble mean, which we refer to as "forecast" even 226 when using delayed-mode observations and atmospheric forcings. The model data has been 227 collocated with the observations for validation. To estimate the forecast differences to 228 observations, we use the standard statistical moments:

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$$Bias = \frac{1}{N} \sum_{i=1}^{N} (H\bar{X}_i - y_i)$$
 (4),

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$$RMSD = \frac{1}{N} \sum_{i=1}^{N} (H\bar{X}_i - y_i)^2$$
 (5),

- Where i is the ith day, N represents the total number of days depending on the
- observations, and  $\mathbf{X}_i$  represents the model daily average at the time of the observation  $y_i$ .
- 233 The  $X_i$  bar denotes the ensemble mean using 100 model members here, and the operator H





extracts the model SSS at the observed location. The model performance can then be quantitatively compared among the three assimilation runs.

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#### 4. Results

4.1 Diagnosing using assimilation statistics

The SSS innovations in the two assimilation runs, ExpV2 and ExpV3, are shown in Fig. 2, together with the number of assimilated SSS observations and the ensemble spread of SSS calculated by the ensemble standard deviation. The total number of observations is maximum in September when the sea ice cover is minimal. Since both versions of the SSS product share the same time frequency (9 days average) and gridded format, the number of assimilated observations in the two runs are identical (gray lines in Fig. 2). For ExpV2, the Root Mean Square (RMS) of the innovation varies between 0.4 and 1.2 psu, but the mean of innovation which is the opposite of the bias (Eq. 1) shows a positive salinity bias, especially during September, when the saline bias is around 0.4 psu. However in ExpV3 the salinity bias quickly disappears after a few data assimilation cycles. The RMS of the innovation are larger in ExpV3 between 0.6 and 1.6 psu, which can partly be explained by the higher effective resolution of the V3.1 product. In ExpV3, the RMS of the SSS innovation (the red line) jumps down after the first SSS assimilation step. The RMS of innovations and the observation errors both decrease from summer to winter, following a yearly cycle as the areas of fresher water get gradually ice-covered. The domain-averaged observation errors are only slightly larger in ExpV3 than in ExpV2, as explained above, and the RMS of innovations become lower than the observation errors near the end of the run, which indicates that the observations errors sound overestimated. Figure 3 shows SSS maps from the two SSS assimilation runs (ExpV2 and ExpV3) and the control run (Exp0) during August and September 2016. For Exp0 in August, low salinity waters are found In the Beaufort Sea near the Mackenzie River and along the East Siberian coast. In September, the low saline waters below 30 psu bridge the two areas in Exp0 probably due to sea ice melt, although the lowest salinity near the Siberian coast remains unchanged from August to September (as indicated by the 28 psu isoline). Both in ExpV2 and ExpV3, the low salinity areas are even fresher during the two months compared to Exp0. Notably, the areas of salinity lower than 28 psu are broader in ExpV3. On the European side of the Arctic, the characteristics of the saline Atlantic water are very similar in all the three runs (as shown by the isolines of 34 and 35 psu in Fig. 3). This is an indication that the model ensemble has a lower standard deviation of SSS and thus less sensitivity to the SSS assimilation in high salinity areas. Furthermore, clear salinity differences are observed in all Arctic marginal seas. The relatively saline tongue in the northwest Laptev Sea indicated by the 32 psu isoline is found in various locations in all three runs. In the Laptev Sea, due to the



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significant effects of river runoff and ice melt, the salinity shows a strong gradient from the southeast to the northern part. During winter, the salinity increases to 34 psu, and decreases in summer near to 30 psu (Janout et al., 2017). In Exp0, the 32 psu salinity tongue extends eastward to Taymyr Peninsula (TP). In ExpV2, the salinity tongue extends eastwards but is narrower, but in ExpV3 it remains to the West of Severnaya Zemlya. North of the TP, the Kara Sea freshwater meets with the Atlantic Water pathways from the Fram Strait and Barents Sea (shown in Figure 1 of Janout et al., 2017). Close to TP, the observations at the mooring profiles in Janout et al. (2017) show much fresher surface salinity (29 psu) than the subsurface salinity (32 psu) in summer. This motivates the assimilation of the SSS products to compensate for the paucity of in-situ observations. The 32 psu isoline in ExpV3 extends hundreds of kilometers further South along east Greenland in comparison to Exp0 and ExpV2. The change between simulations is larger than the differences between August and September. Another area of notable differences is in the northern Baffin Bay. In ExpV3, the area above 32 psu is shrunken to the South of Nares Strait under the assimilation of the V3.1 SSS product, which may compensate for the lack of mass loss from the Greenland ice sheet in the model. In the above comparisons of SSS maps, the central Arctic is excluded, since the region is covered by sea ice and the effect of assimilation can only be indirect. 4.2 Comparison with independent in situ observations Valid observations in the Central Arctic are very unevenly distributed. When pooling all observation types together, we further investigate the SSS misfits separated into six subregions of the Arctic (Fig. 1 and Table 2). This section will present statistics of differences to independent in situ observations considering marginal seas separately. Beaufort Sea: Figure 4 shows the scatterplots of SSS in the three runs against in situ observations which are respectively obtained from BGEP, OMG, and ICES. In the Beaufort Sea (top panel in Fig. 4), the observed SSS varies in a range of 26-29 psu. The range of SSS in Exp0 is much smaller, between 29-31 psu with a saline bias of 2.6 psu and an RMSD of 2.7 psu, but otherwise show a reasonably linear relationship. The SSS bias in Exp0 has the same value as in Xie et al. (2019), although estimated using the BGEP observations in a different time period of 2011-2013. The range of SSS in ExpV2 is slightly improved to 28-30.5 psu, a bias reduction by around 0.5 psu, corresponding to bias and RMSD reductions of respectively 13.5% and 10.5% with respect to Exp0. In ExpV3, the SSS range is much closer, between 26.5 and 30.5 psu, so the bias and RMSD reductions in ExpV3 are

respectively 26.3% and 17.3% with respect to Exp0. Furthermore, compared with the

combined SSS observations shown in the upper of Fig. 6, the SSS misfits in ExpV3 have a





308 robust reduction of 26.0% for bias and 20.6% for RMSD. There is also a reduction in ExpV2 309 of 13.5% for bias and 11.5% for RMSD, but smaller in comparison with ExpV3. These results 310 clearly indicate that assimilating the new version of the SSS is more efficient to improve the 311 SSS in the Beaufort Sea. 312 313 Chukchi Sea: Fig. 5 shows the SSS deviations as a function of time during the SKQ cruise 314 route. Relative to CTD observations, the SSS deviation in the runs are shown as the curves 315 in Fig. 5a. The saline bias (2.8 psu) is more pronounced than in the Beaufort Sea, for which 316 we blame to the climatology relaxation in the Bering Strait where the interannual variability of 317 the Pacific water is not included. After assimilating both SSS products, a gradual reduction of 318 the bias is observed during September, by 15.5% in ExpV2 and up to 22,2% in ExpV3. By 319 the meantime, the comparison to underway surface water samples (Fig. 5b) also shows the 320 error reductions errors around 15%, though less differences between V2 and V3. 321 Furthermore, compared with the combined SSS observations in CS (Fig. 6; bottom panels), 322 the SSS in Exp0 shows a very narrow varied range with a saline bias about 2.3 psu and the 323 RMSD 2.6 psu. A recent observational study by Goñi et al. (2021) shows that the surface 324 salinity of CS during late summer varies around 28-30 psu during 2016-2017 time period. In 325 our analysis for the year 2016, the SSS observations in the region vary around 27-32 psu. 326 through the assimilation of SSS products, the two runs of Exp V2 and ExpV3, show reduced 327 misfits (bias and RMSD). And as expected, the SSS in ExpV3 has more significant reductions in bias (17.7%) and RMSD (16.4%). After assimilation, the deviations are in the 328 329 same range as found in the BS. 330 331 Greenland Sea: Around Greenland, most SSS observations are from OMG shown as the red 332 downward triangles in Fig. 1, distributed around both of the western and easter coastlines. 333 Firstly, compared with all SSS observations from OMG, the SSS misfits in the three runs 334 (shown in the middle panels of Fig. 4 show smaller bias and RMSD if relative to these values 335 in BS and CS. However, the SSS in ExpV3 still shows significant error reductions where the 336 saline bias/RMSD has a reduction of 32.6%/9.4% compared to that in Exp0. Notably, the 337 SSS misfits in ExpV2 are almost the same as in Exp0, which suggests that the V2.0 SSS 338 product loses the benefit around there by DA in this system. 339 To better understand the changes caused by the SSS assimilation and the potential 340 dependence on the localization, we further respectively evaluate the SSS deviations in GS 341 and BB where the involved observations are shown in Fig. 1 (also these two regions are 342 listed as S5 and S6 in Table 2). As shown in the top panel of Fig. 7, the SSS observations in 343 GS vary between 27 and 35 psu. This large SSS variation reflects the real condition: where 344 the fresh Arctic water and the fresh coast water converge with the saltier Atlantic Water. The





three assimilation runs show different saline biases, especially for salinities less than 30 psu. While in observations the minimum salinity is lower than 28 psu, it is around 30 psu in ExpV3, and 31 psu in Exp0 and ExpV2. Correspondingly, the bias reduction in ExpV3 is over 50% with the RMSD decreased about 10.5% in GS. Notably, no clear changes for SSS in ExpV2 are found in comparison with Exp0. As indicated from SSS scatterplots of the three runs in BB (S6 in Table 1, also shown in bottom panels of Fig. 7), there are no clear differences between ExpV2 and Exp0 (less than 0.02 psu). On the other hand, w.r.t ExpV2 and Exp0, ExpV3 registers a reduction of the SSS bias, even has no significant reduction of the RMSD in GS.

Next, we focus on the Barents Sea region (S3 in Table 2) and the Norwegian Sea (S4 in Table 2). The SSS bias and RMSD are the lowest in ExpV3 in Table 2, even though the reductions are not so significant as in the above basins. Compared to the ICES observations distributed in the North Atlantic and extended in Nordic Seas (blue squares in Fig. 1), the scatterplots of Exp0 and ExpV2 are almost similar in the bottom panels of Fig. 4. The minimum salinity in these two runs is higher than 32 psu. The SSS bias and RMSD in both runs are also similar (differences less than 0.01 psu). In contrast, lower saline values in ExpV3, are below 32 psu, although the saline bias remains still around 0.5 psu on average. Notably, the SSS in ExpV3 shows this assimilation brings a bias reduction of 15% compared to Exp0, but the RMSD only reduced about 0.03 psu. It further suggests how to improve the fresh salinity measurements near the coastline around the Nordic Seas will be the next challenge for the SSS retrieve after the V3.1 SSS product.

#### 4.3 Impact analysis of the SSS assimilation

Above quantitative validation of SSS against various observations, shows that the assimilation of these two satellite products brings many positive benefits to constrain the simulated SSS not too far from real conditions, although the improvements are quite dependent on the locations. Surface salinity changes in the three runs (Fig. 8) contrasts the averaged increment of SSS in 2016. The increment means the difference between the analysis model state and the previous forecast model state, and represents the model correction of SSS by DA. As a control reference, the SSS increment in Exp0 is mainly in the river mouths, such as those around the Lena River (LR) and the Yenisey River (YR), while in open ocean it is extremely small. This is an indication that the presently assimilated observations in Exp0 are not able to correct the surface salinity very much. Assimilation of version 2.0 SSS product (Fig. 8b) shows four dominant areas around the central Arctic with negative increment in SSS. Two of them are in the Kara Sea (KS) and the East Siberian Sea (ESS). These are regions where the model has an underestimation for the affected extent of





382 the freshwater impulse around rivers. The third region, the southern Laptev Sea (LS), is 383 found to be further separated into two small areas. The fourth region is along the coastline in 384 Beaufort Sea. On the contrary, a positive increment in SSS is found in the Hudson Bay (HB), 385 outside the central Arctic 386 In comparison to ExpV2, except for the wide negative SSS increment area around ESS, 387 much more areas are found with the different incremental patterns in ExpV3 (Fig. 8c). Two 388 strong positive SSS increment centers appear around the Kara Sea and the north of LS, 389 which is clearly different from the increment pattern in ExpV2. The difference is likely due to 390 the processing of the two versions of the SSS products using different climatologies 391 (Martínez et al., 2022). The two nearby regions (BS coast and HB) with negative SSS 392 increment regions in ExpV2 are found to form a dipole of negative and positive increment 393 regions in ExpV3. This pattern is likely due to the benefits of the increase in the horizontal 394 resolution in the newest version of SSS products. In addition, some regions with positive 395 increment (around 0.1 psu) are also visualized in Fig. 8c, significantly different to that in 396 Exp0: region extending from south of Fram Strait and to north of Denmark Strait; northern 397 Baffin Bay; Chukchi Sea shelf. These spatial features of positive and negative SSS 398 increments in ExpV3 indicate the impact of DA in the Arctic basins. On the other hand, the 399 Barents Sea, Norwegian Sea, and the north Atlantic don't show significant changes due to 400 the SSS assimilation for both runs, which is also consistent with the SSS scatterplots shown 401 in Fig. 4 (bottom panels).

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Since the water salinity near the surface are changed by the SSS DA, it is natural to further investigate how big the impact on the freshwater in the Arctic Ocean. Based on these assimilation runs, the changes in the Freshwater Content (FWC) in the Arctic are calculated according to the method by Proshutinsky et al. (2009), although this method was proposed initially to diagnose the FWC anomalies in the BS:

$$FWCL = \int_{z_2}^{z_1} \frac{[S_{ref} - S_z]}{S_{ref}} dz$$
 (6)

Where the reference salinity value  $S_{\text{ref}}$  is taken at 34.8 psu and the vertical integral is computed from surface on all the waters fresher than  $S_{\text{ref}}$ . Recently, applying the same methodology on optimized interpolation on the collected in-situ observations, Proshutinsky et al. (2020) estimated the time-averaged summer freshwater content in the Beaufort Gyre region for two time-period (1950s-1980s and 2013-2018). They show the FWC centre in BS is located around (150°W, 75°N) and the 20-m isoline covers more than 5 degrees of latitude and nearly 30 degrees of longitude on average. During the recent years (2013-2018), the FWC in BS has an obvious increase compared with before and its centre has a westward shift.





418 Correspondingly, referring to Eq. 6, the FWC of the water column has been computed from 419 surface until the depth reaching to 34.8 psu. Figure 9 shows the FWC around the Arctic on 20<sup>th</sup> September and 20<sup>th</sup> October 2016, respectively. In Exp0, the reanalysis reproduces the 420 421 FWC spread in the Arctic region and a dominant centre located in the Beaufort Sea. Tracking 422 of the 20 m FWCL isolines in Fig. 9a and 9d, it shows an increase in its spatial coverage 423 during October, which verifies the variability due to winds, sea ice conditions, and ocean 424 mixing processes. After assimilation of the V2.0 SSS product, the FWC spatial maximum in 425 BS is found to show a different distribution in Fig. 9b and 9e in comparison to that in Exp0. 426 An increase in FWC is noted outside the BS, north of Canada (indicated by the 16-m isoline). 427 Another noticeable change is the FWCL extending (shown as the 8-m isoline) along the East 428 Siberian shelf and near the coast in the Laptev Sea (LS). It indicates that the SSS 429 assimilation is able to correct the possible fresh bias related to the river fluxes in the model near the coastal regions in ESS and LS. In ExpV3, the FWC on the shelf region of ESS is 430 431 higher compared to that in ExpV2, but lower near the southwest coast of LS. These results 432 suggest that the SSS assimilation of both versions of satellite products will redistribute the 433 freshwater in the Arctic, and the freshwater budget will be adjusted in the end. However, so 434 far with the limited amount of in-situ data, it is not fair to conclude whether this is a change 435 for the better or the worse. Significantly different from sparse in-situ observations in the 436 Arctic, the reanalysis product can better represent the characteristics of FWC variations in 437 space and time. 438 Further, we intercompare the daily time series of FWCL from the three runs averaged over 439 north of 70°N (Fig. 10). The averaged FWCL clearly shows a sharp increase till October-440 November to reach the maximum, and gradually decreases thereafter. The impact of weekly 441 data assimilation cycles is visible as instantaneous jumps on the three curves of the time 442 series. The summer FWC is found to increase substantially due to SSS assimilations in 443 ExpV2 and ExpV3. Notably the assimilation of version 3.1 SSS brings faster increase during 444 the first two months. Since there is not enough ground truth data in 2016, the above 445 comparison can only be qualitative, but the timing is in better agreement with the ITP data 446 presented by Rosenblum et al. (2021, their Fig. 4), although the amplitude of the seasonal FWC seems too small in all experiments, which can be related to insufficient thick ice in 447 448 TOPAZ4 (Uotila et al., 2019). More concrete evidence about the changed FWC will be 449 provided, after when the longer assimilation of the satellite-based SSS product is finished in 450 near future.

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## 5. Summary and discussions.





453 SSS plays a key role to track the water property in the global water cycle and the ocean 454 dynamics, but hindered by the extreme paucity of in situ data, the Arctic SSS still has high 455 uncertainty. As a promising tool to measure the SSS changes in Arctic at basin scale, the 456 grided SSS products from SMOS undoubtedly provide a way constraining the salinity 457 deviations, especially for the ocean forecast systems. However, due to the limits of the 458 previous SSS products, there have not been any previous studies to investigate the real 459 benefits or challenges for assimilation of SMOS SSS in the Arctic reanalysis. In this study, 460 based on the coupled ice-ocean data assimilative system, three assimilation runs have done. 461 Exp0 assimilated all available altimeter data, SST, sea ice concentration, sea ice drift, T/S 462 profiles, sea ice thickness, except any SMOS SSS products. ExpV2 and ExpV3 additionally 463 assimilated V2.0 and V3.1 of SSS products from BEC, which were tested and retrieved by a 464 series of algorithms considering the low temperature and sea ice cover in the Arctic (Olmedo 465 et al., 2017; Martínez et al., 2022). 466 Evaluated by the independent SSS observations from CTD and surface water samples along 467 the cruise underway, the quantitative misfits in ExpV2 and ExpV3 have been significantly reduced relative to that in Exp0. In the Beaufort Sea, the SSS bias and RMSD in ExpV3 is 468 reduced respectively by 26.0% and 20.6%, and if validated only against the observations 469 470 from BGEP, the reduction is up to 26.3% and 17.3% respectively (Fig. 4). For ExpV2, the 471 RMSD is reduced by 11.5% (if validated against the BGEP CTD profiles about 10.5% in Fig. 472 4). In the Chukchi Sea, the reduction in SSS misfits in ExpV3 (bias:17.7%; RMSD: 16.4%) is 473 more than that in ExpV2 (bias: 15.5%; RMSD: 13.7%). Around Greenland, validated by the 474 SSS observations from OMG, a significant reduction in the SSS bias (32.6%) and RMSD 475 (9.4%) is found in ExpV3, while there is no notable improvement in ExpV2. Furthermore, 476 dividing the observations around Greenland into two regions, S5 and S6 (Table 2 and Fig. 7) show a larger reduction in the bias (52%) and RMSD (10.5%) in the Greenland Sea (S5) in 477 478 ExpV3 SSS relative to that in Exp0. Notably in the Baffin Bay (S6), only the SSS bias in 479 ExpV3 shows an obvious reduction compared with Exp0. It is consistent with the markable 480 adjustment along the 34 psu isoline near the ice edge in GS (shown in Fig. 3). Increments of 481 SSS (in Fig. 8) also clearly show the wide salty features located in the GS in ExpV3, which is 482 clearly different to that in Exp0 and ExpV2. In addition, the increments for other variables 483 such as SST, SIC and so on are diagnosed, but their spatial features during the same time 484 (figures not shown) have no clear differences as in Exp0. It further verifies the surface salinity 485 is dominantly constrained by the direct observations from SMOS, other than the weak 486 constraints through the error covariance from other observed variables. This finding also is 487 consistent with the conclusions in SSS assimilation experiments in the tropics (Chakraborty 488 et al.,2015; Tranchant et al.,2019).





490 Furthermore, this study shows that the error reduction of SSS will be benefited from the 491 assimilation of the V3.1 product from SMOS, even outside of the central Arctic. A remarkable 492 improvement is also achieved around GS (S5 in Fig. 1), a clear advantage compared to the 493 other version of SSS product. Moreover, our analysis shows different spatial distributions of 494 Arctic FWC as a result from assimilating the two SMOS products respectively. The mean 495 FWCL north of 70°N shows that the FWC in the whole central Arctic can be corrected by the 496 SSS innovations though DA, although the FWCL time series shows a clear step jump for 497 each assimilation cycle. Assimilation experiments show that the Arctic FWC can be 498 redistributed by assimilation, but how the seasonal cycle varies with time still needs a longer 499 assimilation time. Clearly, these novel results are not only useful for the developing of the 500 Arctic reanalysis and the operational ocean forecast system, but also provides insights for 501 understanding the differences of these two SSS products although they have a certain 502 degree of similarity. These results are also expected to guide the future upgrade of the SSS 503 products. 504 505 Using the quantitative SSS misfits (Table 2), the impact indexes at each subregion (S1 to S6) 506 further indicates whether the misfits are significantly decreased or not. Outside of the central 507 Arctic, the v2.0 SSS product loses the impacts in this system, but the V3.1 SSS brings more 508 wider significant impacts around the Arctic, which clearly benefits from the related retrieval 509 algorithms for the refined effective resolution (Martínez et al., 2022). However, in the region 510 S6, the SSS in ExpV3 has no significant constraint on the misfits and only brings a reduction 511 in the bias. It may be related with the movement of the sea ice edge more northward in 512 summer and indicates that both the SSS products have low impacts over the open water in 513 the north Atlantic. It is also verified by the validation results in the Barents Sea and the 514 Norwegian Sea, as shown in bottom panels of Fig. 4 and Table 2. This defect partly reflects 515 the mesoscale eddy features (<50 km which is about 4 times the model resolution in 516 TOPAZ4) having no clear benefits from this assimilation using the 9-days SSS. In fact, the 517 V3.1 SSS also provides a 3-days product that needs to be tested by DA for quantifying the 518 impact on the north Atlantic. Meanwhile, considering the coarse footprint of the SMOS 519 radiometer (about 40 km in diameter), minimal sampling densities (e.g., Lv et al., 2020) is 520 required to resolve the mesoscale eddy features. But in real conditions the gridded SSS 521 products still have a gap for more precisely measuring the SSS changes near the Nordic 522 coast regions. Using the same L-band frequency (e.g., Lee et al, 2012), Aquarius used three 523 radiometers at fixed angles and had a 350 km wide swath that covered earth's surface in 524 seven days. Whereas SMAP scans earth using a spinning antenna, with a wider swath about 525 1000 km every three days to provide global coverage (e.g., Tang et al., 2017; Reul et al., 526 2020). To combine all the SSS retrieves along the satellite tracks will provide the





527 contemporaneous data coverage with the greatest extent, which should be helpful in Arctic 528 and high-latitudes for further improvements of the reanalysis and the ocean forecasting. 529 530 Data availability. All the in situ observations for validation in this study are open accessed 531 as the states in Sect. 3. The model result in Exp0 same as the released reanalysis from 532 TOPAZ4 which is freely available from CMEMS (http://marine.copernicus. eu). Other two 533 assimilation data can be freely provided for public by personal communication. 534 535 **Author contributions.** JX initiated the design and carry of the assimilation experiments. 536 LB and RR contributed the result interpretation. JC collected the SSS data. CG and RC 537 enhanced the understanding for the uncertainty of the satellite data. All the authors 538 contribute to edit and correct this paper. 539 540 **Competinginterests.** The authors declare that they have no conflict of interest. 541 542 Acknowledgments: 543 Thanks to the profile data providers: the OMG mission for the released final CTD data via 544 the Physical Oceanography DAAC (PO.DAAC); the ICES data portal (https://www.ices.dk); 545 the Arctic Data Center (https://arcticdata.io/catalog/data); and the BGEP data were available 546 based at the Woods Hole Oceanographic Institution 547 (https://www2.whoi.edu/site/beaufortgyre/) in collaboration with researchers from Fisheries 548 and Oceans Canada at the Institute of Ocean Sciences. This study has been supported by 549 the ESA Arctic Salinity+ project and by the NFR Thickness of Arctic sea ice Reconstructed 550 by Data assimilation and artificial Intelligence Seamlessly (TARDIS) project. The computation 551 of the assimilation experiments and the plotting of the results were performed on resources 552 provided by Sigma2-the National Infrastructure for High Performance Computing and Data 553 Storage in Norway with the projects of nn2293k and nn9481k and the relevant store space 554 under the projects of ns9481k and ns2993k. 555 556 Reference: 557 Bouillon, S., Fichefet, T., Legat, V., and Madec, G.: The elastic-viscous-plastic method revised, 558 Ocean Modell., 7, 2–12, https://doi.org/10.1016/j.ocemod.2013.05.013, 2013.





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## Caption and figures:

Table 1. Settings of the three assimilation runs in 2016 with and without SSS.

	Assimilated obs.	Initial model states	End date of assimilation	SSS Observation Errors
Exp0	SST, SLA, T/S profile, SIC, SIT, and SID	6 <sup>th</sup> July	28 <sup>th</sup> Dec.	N/A
ExpV2	SSS V2.0 + obs. used in Exp0	6 <sup>th</sup> July	28 <sup>th</sup> Dec.	Eq. 3
ExpV3	SSS V3.1 + obs. used in Exp0	6 <sup>th</sup> July	28 <sup>th</sup> Dec.	Eq. 3

**Table** 2. Evaluation of SSS misfits (unit: psu) in the three assimilation runs according to the 6 sub-regions indicated by the blue dashed lines in Fig. 1. The bold fonts indicate the minimal misfits in the runs with a significant reduction (> 9% with respect to Exp0). The overall score is defined by whether the reductions of bias and RMSD are significant or not. If both reductions are significant, the index equals 1, but 2 if only one of them is reduced, and otherwise equals 3.

Regio	Areas in Fig. 1	Numbe r of	Bias (psu)		RMSD (psu)			Overall score		
n		obs.	Ехр	ExpV	ExpV	Exp	ExpV	ExpV	ExpV	ExpV3
			0	2	3	0	2	3	2	
S1	BS	98	2.81	2.43	2.08	2.87	2.54	2.28	1	1
S2	CS	137	2.32	1.96	1.91	2.62	2.26	2.19	1	1
S3	BSS	189	1.35	1.34	1.30	2.50	2.49	2.47	3	3
S4	NS	669	0.43	0.44	0.37	1.19	1.19	1.16	3	2
S5	GS	254	0.50	0.51	0.24	1.43	1.43	1.28	3	1
S6	BB	89	0.35	0.37	0.12	1.22	1.20	1.22	3	2





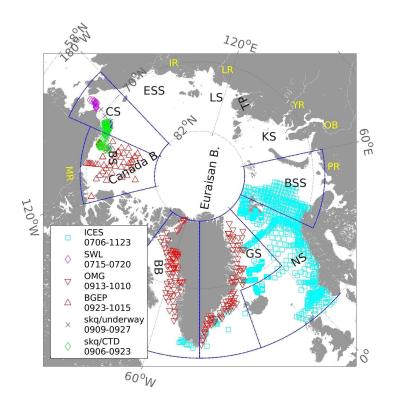
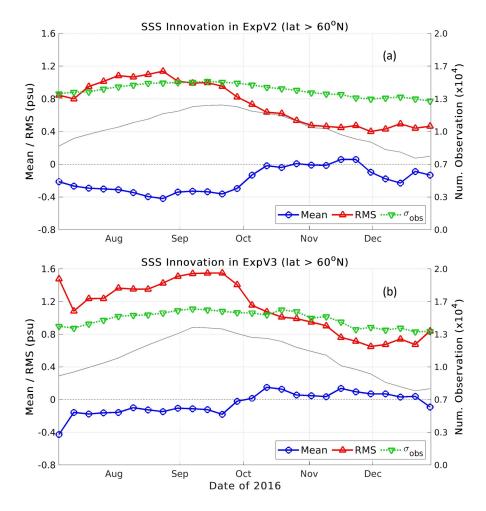


Fig. 1 Locations of the observed SSS from in-situ profiles and surface samples by cruises from July to December 2016. There are 6 observation sources noted by the marks, see the details in Section 2.3. The marginal seas delineated are the Beaufort Sea (BS), Chukchi Sea (CS), East Siberian Sea (ESS), Laptev Sea (LS), Kara Sea (KS), Barents Sea (BSS), Greenland Sea (GS), Norwegian Sea (NS), and Baffin Bay (BB). The main rivers around the Arctic region are the Mackenzie River (MR), Pechora (PR), the Ob (OB), Yenisey River (YR), Lena River (LR), and Indigirka River (IR). TP indicates the Taymyr Peninsula.



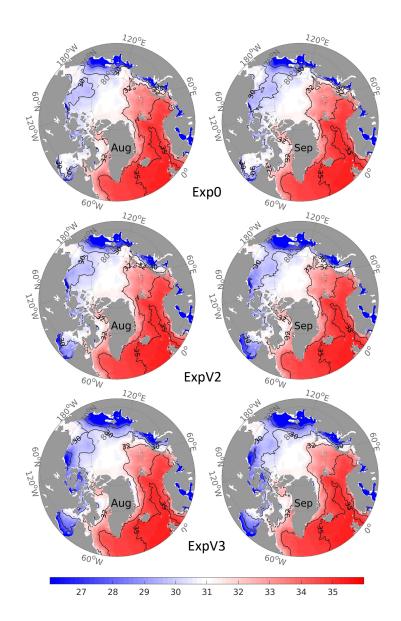




**Fig** 2. Innovations of SSS in both weekly assimilation runs ExpV2 (a) and ExpV3 (b). The line with red triangles is the root mean squared innovation, and the blue dotted line shows the mean of innovations north of 60°N. The gray line represents the number of observations assimilated, and the line with inverted triangles is the observation error standard deviation in the two runs.



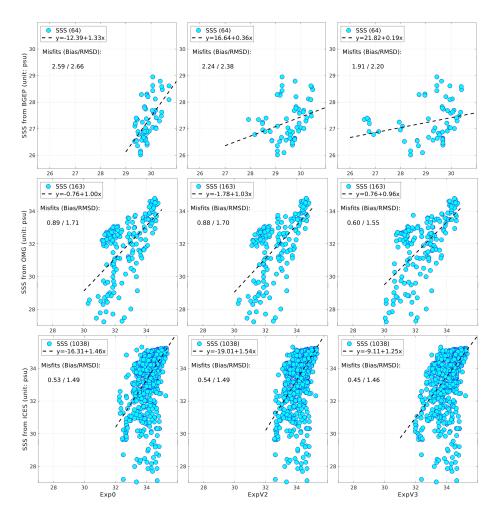




**Fig.** 3 Monthly simulated SSS (unit: psu) in August (left column) and September (right column) 2016 from Exp0 (top line), ExpV2 (middle line), and ExpV3 (bottom line). The black isolines indicate the 28, 30, 32, 34 and 35 psu isolines.



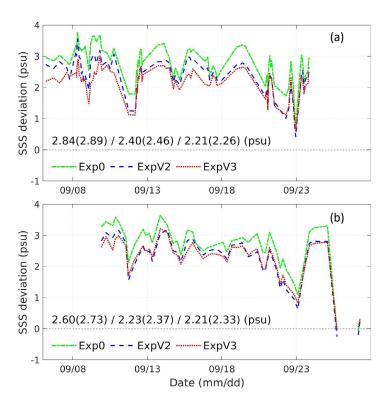




**Fig.** 4 Scatterplots of SSS in the TOPAZ assimilation runs against in-situ profiles (Upper: from BGEP in the Beaufort Sea; Middle: from OMG in both Greenland Seas; Bottom: from ICES in the Nordic Seas as indicated in Fig.1 and descriptions in 2.1). The statistics of SSS misfits are indicated in each panel with the bias and the RMSD respectively, the number of observations is given between parentheses, and the dark dashed line represents the linear regression.



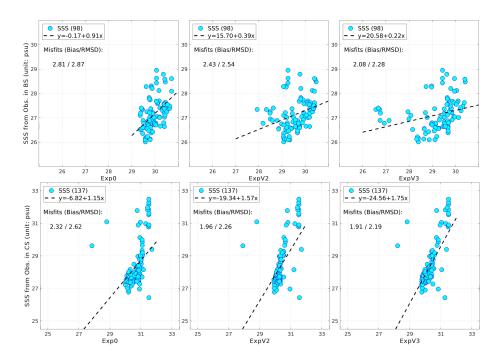




**Fig.** 5 Model-minus-observations SSS differences in the three assimilation runs against the SSS recorded in the Beaufort Sea and the Chukchi Sea along the SKQ cruise in 2016: a) from CTD profiles; b) from surface water samples underway in the same cruise. The biases are indicated in the same order and the corresponding RMSD between parentheses.



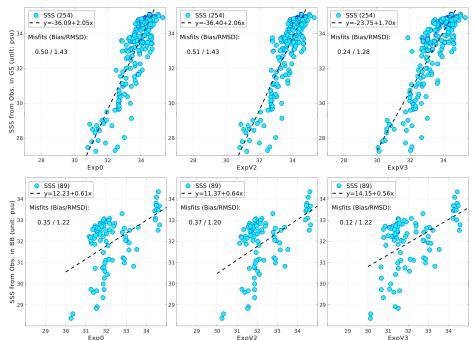




**Fig.** 6 Scatterplots of SSS (unit: psu) in the three assimilation runs of Exp0, ExpV2 and ExpV3 against the observations from the CTD profiles collected by different cruises in 2016. **Upper**: in the Beaufort Sea; **Bottom**: in the Chukchi Sea as shown in Fig.1.



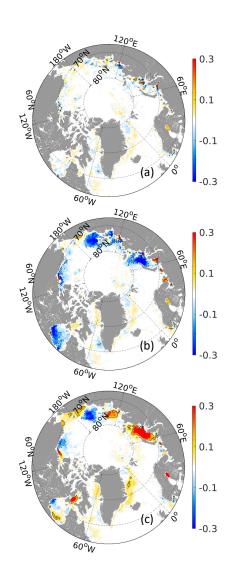




**Fig**. 7 Scatterplots of SSS (unit: psu) in the three assimilation runs of Exp0, ExpV2 and ExpV3 against the collected observations with the CTD profiles from OMG and ICES in 2016. **Upper**: in the Greenland East Sea; **Bottom**: in Baffin Bay as shown in Fig.1.



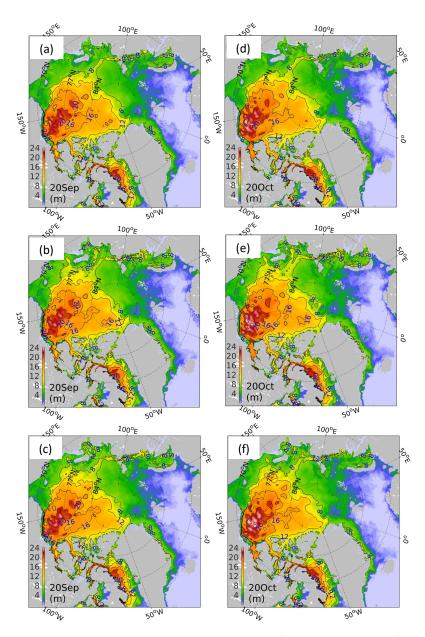




**Fig** 8. Averaged increment of SSS in Exp0 (a), ExpV2 (b) and ExpV3 (c). The obvious changes of SSS (±0.1 psu) are highlighted by isolines.



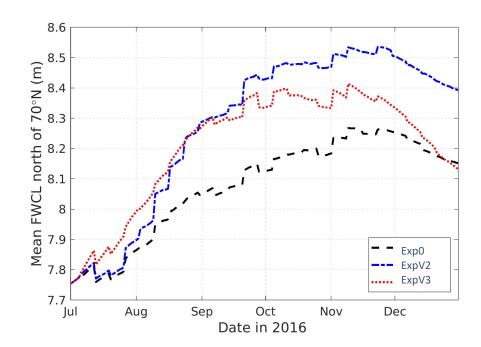




**Fig** 9. Daily freshwater content depths (unit: m) on 20<sup>th</sup> September and 20<sup>th</sup> October 2016 in Arctic Ocean from the three assimilation runs: Exp0 (a; d), ExpV2 (b; e), and ExpV3 (c; f). The interval of isolines is 4 meters.







**Fig** 10. Mean freshwater content depths (unit: m) in the central Arctic (>70°N) during the period from July to December 2016 for Exp0 (dark dashed), ExpV2 (blue dashed), and ExpV3 (red dotted).