Determination of the Sea Surface Salinity Error Budget in the Soil Moisture and Ocean Salinity Mission

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Abstract—The Soil Moisture and Ocean Salinity mission will provide sea surface salinity maps over the oceans, beginning in late 2009. In this paper an ocean salinity error budget is described, an analysis needed to identify the magnitude of the error sources associated with the retrieval. Instrumental, external noise sources, and geophysical errors have been analyzed, stressing their relative impact. This paper includes results from previous studies, addressing the impact of multisource auxiliary sea surface temperature and wind speed data on the final salinity error. It provides, moreover, a sensitivity analysis to the uncertainty of the auxiliary salinity field. Salinity retrieval has been addressed in a wide set of configurations of the inversion algorithm.

Index Terms—Error budget, retrieval, salinity, Soil Moisture and Ocean Salinity (SMOS).

I. INTRODUCTION

GLOBAL measurements of sea salinity will provide direct insights on the relationships and feedback between oceans and climate. Salinity fields and their seasonal and interannual variability are at the same time tracers and constraints on the water cycle and on coupled ocean–atmosphere models. Despite the recent deployment of the ARGO-buoys system over most of the global oceans, an in situ time series is still lacking [1]. As a matter of fact, this dearth of salinity measurements may result in major discrepancies between modeled and observed surface currents and in estimates of the evaporation/precipitation balance. Accordingly, the major outcome of a satellite mission for salinity monitoring would be to provide this information globally and synoptically. Knowledge on a number of highly relevant phenomena can be gained for large-scale oceanography and climatology using this spaceborne observational approach.

The European Space Agency’s Soil Moisture and Ocean Salinity (SMOS) mission will provide global sea surface salinity maps over the oceans, beginning in late 2009. These maps will be available with frequent temporal coverage, addressing the link among the water cycle, ocean circulation, and climate [2]. SMOS’s single payload is the Microwave Imaging Radiometer by Aperture Synthesis (MIRAS), which is a novel L-band radiometer that makes use of 2-D aperture synthesis interferometry to measure the brightness temperature ($T_B$) at two orthogonal polarizations within a wide field of view (FOV) [3]. The MIRAS instrument has multiantangling imaging capability as the satellite moves over the Earth. Microwave radiometric measurements, in the band of 1400–1427 MHz, provide the suitable observables for salinity estimation. This protected band is a compromise among brightness temperature sensitivity to salinity, little interference due to the atmosphere, and reasonable pixel resolution.

The SMOS ocean community is currently working toward the determination of a robust inversion scheme to enable SSS retrievals (the so-called level 2 data) from brightness temperature data. The established requirements are very challenging: 0.1 practical salinity unit (psu) accuracy over $2^\circ \times 2^\circ$ grid cells in one month [4]. Despite the nearly optimal conditions to retrieve salinity from L-band microwave radiometry, the sea surface salinity signature in brightness temperature is still rather small. Hence, efforts are required to achieve excellent instrument performance and calibration, as well as an optimum definition of the geophysical parameter retrieval scheme.

The salinity retrieval issues that are critical to the inversion procedure are the following:

1) scene-dependent bias in the simulated measurements;
2) radiometric errors (associated with thermal noise or imperfect instrument and calibration);
3) L-band forward geophysical model function (GMF) definition;
4) auxiliary data, namely, sea surface temperature ($SST$) and wind speed ($U_{10}$), collocation, and uncertainties;
5) constraints in the cost function, particularly in the salinity term;
6) adequate spatio-temporal averaging.

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To support this, a comprehensive salinity error budget analysis has been developed. The objective is to identify the relative impact of the various aspects of the retrieval and to ultimately establish a hierarchy of the issues to be tackled in the SSS retrieval scheme. The basic approach is to propagate and quantify the instrumental, geophysical, or external noise source errors as spatio-temporally averaged salinity errors (the so-called level 3 product).

II. SEA SURFACE SALINITY RETRIEVAL

Sea surface salinity retrieval requires the knowledge of various geophysical and environmental factors to properly process the radiometric measurements. Its complexity is related not only to the narrow range of ocean brightness temperatures but also to the signatures of other geophysical parameters in the measured values (such as sea state/roughness), which are stronger than the salinity signal.

A robust inversion scheme implemented for SMOS SSS retrieval from radiometric estimates is based on the Levenberg–Marquardt iterative numerical algorithm [5], which compares the satellite measured $T_B$ with the values provided by an L-band forward model. This algorithm implements a cost function in which the error $\varepsilon$ (variance) between the modeled and measured data at all incidence angles $\hat{\theta}$ is minimized for each overpass to obtain a set of estimated parameters ($\hat{P} = [\hat{SSS}, SST, U_{10}]$) [6]

$$\varepsilon = \frac{1}{N_{\text{obs}}} \sum_n \left\{ \left[ F_{\text{model}}(\theta, \hat{P}) - F_{\text{data}}(\theta, \hat{P}) \right]^T \overline{C}^{-1} \left[ F_{\text{model}}(\theta, \hat{P}) - F_{\text{data}}(\theta, \hat{P}) \right] + \frac{(\hat{SSS} - SSS_{\text{ref}})^2}{\sigma_{\text{SSS}}^2} + \frac{(SST - SST_{\text{ref}})^2}{\sigma_{\text{SST}}^2} + \frac{(U_{10} - U_{10,\text{ref}})^2}{\sigma_{U_{10}}^2} \right\}$$

(1)

where $N_{\text{obs}}$ the number of observations acquired in a single pixel during a satellite overpass, which depends on the pixel’s distance from the satellite’s ground track. As the distance increases, the pixel is imaged fewer times, and the angular variation is reduced. The instrument’s noise increases, with correspondingly degraded performance in terms of the quality of the retrieved parameters;

the error covariance matrix that depends on the SMOS operation mode (fully polarimetric or dual polarization [7]), the reference frame (Earth or antenna), and the pixel position in the FOV [6];

$\overline{C}$ a vector that contains the modeled or the measured observables. The structure of $F$ depends on the formulation of the retrieval problem, which may be versatile (antenna reference frame, Earth reference frame, or first Stokes parameter formulation), provided that the appropriate corrections are applied;

reference auxiliary data variances.

The first term of (1) includes the measured $T_B$ (the observables; though simulated, so far) and the modeled ones, while the subsequent terms are the so-called background terms and represent constraints applied to ease the convergence of the algorithm based on physical a priori information.

A maximum-likelihood Bayesian approach is used [8], [9], taking advantage of this a priori information available about geophysical parameters. The auxiliary data variances are used to properly weigh the cost function terms according to the accuracy of the quantity being estimated. In fact, the influence of the a priori reference values depends on the uncertainty of these values.

A first-guess salinity value is iteratively modified until an optimal fit is found with the measured $T_B$ while satisfying the geophysical constraints [10]. The overdetermination of multi-look SMOS capabilities is exploited here; the larger the number of observations of a single pixel is (up to 78 per polarization in the central part of the FOV), the better the fit will be to estimate the SSS in this pixel.

A key aspect that has to be recognized is the fact that different algorithm settings and assumptions lead to different retrieval performances. In this paper, the error budget study has been conducted using two configurations of the cost function. Referring to (1), the first configuration considers all the background terms ($SSS, SST,$ and $U_{10}$) as constraints (hereafter “constrained configuration”), while the second lets only the salinity be a free parameter, neglecting its background constraint (hereafter “nonconstrained configuration”).

III. METHODOLOGY AND SIMULATION FEATURES

An error budget study allows the evaluation of the impact of specific error sources in the SSS retrieval performances. A significant characteristic of this study is that all simulations have been carried out by using the SMOS End-to-end Performance Simulator (SEPS) Simulator [11]. Brightness temperature maps generated by SEPS have realistic biases induced by residual calibration errors of the noise injection radiometer (NIR) and by the image reconstruction algorithm, as well as the pixel-dependent radiometric accuracy. The SEPS simulator has been used in its “light” version (i.e., the visibilities have been computed by means of an FFT, considering all the antenna patterns to be identical). All other instrument errors and residual
calibration errors are, in turn, taken into account. This provided substantial savings in computational time, but it unavoidably introduced some approximations, to the detriment of the full characterization of the instrument features. For simplicity, the simulations have been run without radiometric noise, except otherwise specified.

The Universitat Politècnica de Catalunya level 2 processor software package is, in turn, used to control the submodules of the salinity retrieval scheme. Moreover, the level 2 processor is in charge of performing the bias mitigation/cancellation of the brightness temperatures coming from SEPS [12].

The geographic area selected for simulation comprises $10^\circ \times 10^\circ$ in the Mid-Atlantic Ocean (longitude $35^\circ W - 25^\circ W$, latitude $35^\circ N - 45^\circ N$). Month-long simulations have been considered, propagating and then averaging the corresponding overpasses over the selected area. The satellite ascending passes have been selected, and simulations have been performed in the SMOS baseline configuration (dual-pol). Retrieval has been performed both in the antenna reference frame ($Tx$ and $Ty$, to avoid singularities in the transformation from the antenna to the Earth reference frame) and by using the first Stokes parameter ($I$). The baseline semiempirical model considered in the simulations is a piecewise linear fit to the Hollinger measurements [13], while the dielectric constant is parameterized using the Klein and Swift model [14].

It is fundamental to emphasize that the master scenario and the subsequent overall simulation scheme have been conceived using constant geophysical inputs and auxiliary data. The chosen values are: 35 psu for the salinity, 15 °C for the SST, and 10 m/s for the wind speed. The salinity constraint uncertainty in the cost function ($\sigma_{SSS}$) is set to 0.5 psu. This value has been arbitrarily chosen but is physically consistent, as will be discussed in Section V. A sensitivity study of the retrieved SSS performance with respect to the value of $\sigma_{SSS}$ will be discussed as well, and it represents one of the new aspects of this study. Concerning SST and $U_{10}$, the values of the expected uncertainties in the cost function $\sigma_{SSS}$ and $\sigma_{U_{10}}$ are 0.5 °C and 1.5 m/s, respectively.

Fig. 1 shows a flowchart of the end-to-end simulation and processing chain. Single-overpass level 2 SSS values are first temporally averaged in a single-grid cell. This is performed using a weighting procedure which takes into account the pixel position in the SMOS FOV in each overpass, giving less weight to the noisy observations away from the satellite’s ground track. Therefore, these monthly averaged pixels are spatially averaged in a $2^\circ \times 2^\circ$ grid. The distribution of the corresponding error over the selected $10^\circ \times 10^\circ$ test area provides the retrieval performances, which are reported as mean misfit, accuracy (standard deviation), and rms of the error.

Following the approach of [15], in the context of the Aquarius mission, an attempt has been made to provide an SMOS error budget table [16]. For clarity, error sources have been binned into the following:

1) instrument and image reconstruction algorithm errors;
2) external noise sources (Faraday rotation and Sun contamination);
3) geophysical (auxiliary data) errors.

Each of these items will have a certain amount of impact on the SSS retrieval scheme, and the various contributions to the final error in SSS at level 3 will be separately analyzed. To this end, a master scenario has been created to define a simulation baseline over which the comparisons of the error budget study will be performed with an imposed hierarchy. A simulation with the features described in Fig. 1 will be performed for each specific item that will be taken into account in the error budget. It should be stressed that the errors are provided at level 3 (spatio-temporal average) to be consistent with the mission requirements and to propagate various effects that have been studied at level 1, whose final SSS error contributions were
unknown. Moreover, the single-overpass level 2 results are combined using a straightforward weighted average procedure, which ensures homogeneity in the pixel sampling among satellite overpasses. In turn, it is known that other specific techniques are suitable to optimally average the data or separate different spatial regimes. At this stage, the application of any of these techniques is outside the scope of this paper, but further work may be performed to extract further information from these results.

IV. SALINITY RETRIEVAL ERROR BUDGET

As stated in Section II, the error budget study has been performed in both “constrained” and “nonconstrained” algorithm configurations [16], since whether constraints on SSS need to be included is still a matter of debate. In Tables I and II, the outputs of both master scenarios define the performances of the level 3 retrieval. They are provided as mean misfit in the selected zone, accuracy, and rms error, with the last representing the most relevant statistic. It has to be recalled that, in Table I, the master scenario is a baseline simulation with $\sigma_{SSS} = 0.5$ psu. In the following sections, each item under study is evaluated by selective comparison with these baseline scenario outputs. Concerning mean misfits, the results are the relative algebraic differences; in turn, the accuracy and the rms are the quadratic differences from the master scenario results.

A. Instrumental Error Sources

The first class of errors arise at level 1 (brightness temperature maps), deriving from instrumental features and from the image reconstruction algorithm. A typical distinction is made between two radiometric noise sources: the radiometric

| TABLE I |

**ERROR BUDGET—CONSTRAINED SALINITY RETRIEVAL CONFIGURATION**

<table>
<thead>
<tr>
<th>Items</th>
<th>Mean misfit (psu)</th>
<th>Accuracy (psu)</th>
<th>RMS (psu)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$T_x/T_y$</td>
<td>$\sigma$</td>
<td>$T_x/T_y$</td>
</tr>
<tr>
<td>Instrument and Image Reconstruction Algorithm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Master scenario</td>
<td>0.055</td>
<td>0.060</td>
<td>0.031</td>
</tr>
<tr>
<td>2. Radiometric resolution</td>
<td>-0.001</td>
<td>0.000</td>
<td>0.011</td>
</tr>
<tr>
<td>External Sources</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. Faraday rotation</td>
<td>0.001</td>
<td>N/A</td>
<td>0.014</td>
</tr>
<tr>
<td>4. Residual Sun, Max $T_B$</td>
<td>0.004</td>
<td>0.017</td>
<td>0.018</td>
</tr>
<tr>
<td>5. Total error budget flat surface</td>
<td>0.059</td>
<td>0.077</td>
<td>0.040</td>
</tr>
<tr>
<td>Geophysical Sources</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6. Auxiliary SST</td>
<td>0.092</td>
<td>0.003</td>
<td>0.026</td>
</tr>
<tr>
<td>7. Total error budget auxiliary SST</td>
<td>0.061</td>
<td>0.080</td>
<td>0.048</td>
</tr>
<tr>
<td>8. Auxiliary wind</td>
<td>-0.029</td>
<td>-0.076</td>
<td>0.217</td>
</tr>
<tr>
<td>9. Total error budget auxiliary wind</td>
<td>0.032</td>
<td>0.004</td>
<td>0.222</td>
</tr>
</tbody>
</table>

| TABLE II |

**ERROR BUDGET—NONCONSTRAINED SALINITY RETRIEVAL CONFIGURATION**

<table>
<thead>
<tr>
<th>Items</th>
<th>Mean misfit (psu)</th>
<th>Accuracy (psu)</th>
<th>RMS (psu)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$T_x/T_y$</td>
<td>$\sigma$</td>
<td>$T_x/T_y$</td>
</tr>
<tr>
<td>Instrument and Image Reconstruction Algorithm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Master scenario</td>
<td>0.673</td>
<td>0.543</td>
<td>0.396</td>
</tr>
<tr>
<td>2. Radiometric resolution</td>
<td>-0.015</td>
<td>0.001</td>
<td>0.152</td>
</tr>
<tr>
<td>External Sources</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. Faraday rotation</td>
<td>0.009</td>
<td>N/A</td>
<td>0.157</td>
</tr>
<tr>
<td>4. Residual Sun, Max $T_B$</td>
<td>0.107</td>
<td>0.136</td>
<td>0.253</td>
</tr>
<tr>
<td>5. Total error budget flat surface</td>
<td>0.774</td>
<td>0.680</td>
<td>0.518</td>
</tr>
<tr>
<td>Geophysical Sources</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6. Auxiliary SST</td>
<td>0.002</td>
<td>0.003</td>
<td>0.026</td>
</tr>
<tr>
<td>7. Total error budget auxiliary SST</td>
<td>0.776</td>
<td>0.683</td>
<td>0.519</td>
</tr>
<tr>
<td>8. Auxiliary wind</td>
<td>-0.029</td>
<td>-0.076</td>
<td>0.217</td>
</tr>
<tr>
<td>9. Total error budget auxiliary wind</td>
<td>0.747</td>
<td>0.607</td>
<td>0.562</td>
</tr>
</tbody>
</table>
accuracy, which represents a spatial pixel-by-pixel random noise, and the radiometric resolution, which is, in turn, a temporal random noise of a given pixel.

The salinity mean misfits for the master scenario in the constrained configuration are 0.055 psu in $T_x$ and $T_y$ retrieval (antenna reference frame) and 0.060 psu using $I$ (first Stokes parameter). The corresponding results for the nonconstrained configuration are 0.673 and 0.543 psu, respectively. These are residual offsets that have not been removed even though the level 2 bias mitigation algorithm has been applied [12], [17]. It has to be noticed that these offsets are dependent on the extent of the test area and on the SMOS sampling pattern and cannot be assumed as systemic global biases.

It needs to be mentioned that, when dealing with realistic simulations, a fairly large bias of 1.5–2 K is still present in the $T_B$ measurements. This systematic level 1 bias is mainly caused by imperfect calibration and/or drifts in the NIR, besides the image reconstruction algorithm itself. This so-called scene-dependent bias has been thoroughly studied and quantified in the past few years, and techniques have been devised to mitigate it. Bias can seriously jeopardize the salinity retrieval. Nevertheless in the open ocean it is lower and fairly constant within the FOV. Recently, new bias mitigation techniques have been devised, lowering the average bias in a FOV down to 1–1.5 K or less [18], [19]. The salinity mean misfits reported earlier represent, therefore, the propagation of this effect after spatio-temporal averaging.

For the master scenario, in which almost all the possible sources of errors are isolated, salinity accuracy cannot be any better than 0.031 and 0.042 psu for the constrained configuration and 0.396 and 0.370 psu for the nonconstrained configuration for $T_x/T_y$ and $I$, respectively. It has to be recalled that these scenarios have been simulated in the radiometric ideal case (without thermal noise), but with quasi-realistic instrumental features. The results indicate that the retrieval dramatically worsens as the minimization setting is moved toward the nonconstrained configuration. This constitutes the worst case scenario that will define the upper-bound value of the salinity retrieval. Fig. 2 shows the histogram of the nonconstrained weighted master scenario $T_x/T_y$ retrieval, showing the distribution of the $2^\circ \times 2^\circ$ spatio-temporally averaged errors over the $10^\circ \times 10^\circ$ test area.

The contribution of the radiometric resolution (thermal noise) is estimated from realistic calculations made using SEPS, which consider the degradation toward the swath edges. This is the only set of simulations run with radiometric thermal noise. The comparative effect has been studied considering the nominal integration time ($\tau = 0.158$ s), as established in the technical specification of the mission. This should not be confused with the nominal time interval between snapshots, which will be 1.2 s per polarization.

As expected, the relative mean misfit is negligible in both configurations due to the nature of this random noise. The quantitative rms effect of radiometric sensitivity ranges from 0.004 to 0.021 psu in the constrained configuration and from 0.056 to 0.198 psu in the nonconstrained configuration. The ratio of the thermal noise accuracy contribution to the master scenario in the latter case is similar to the constrained configuration case.

The following part of this error budget analysis aims at investigating the potential Sun contamination of the SMOS measurements. Despite the fact that direct Sun contamination involves a relatively small percentage of pixels in any given instantaneous FOV, failure to correct it would have a strong impact on the results.

The Sun’s impact was originally addressed by considering the corresponding average radiometric noise degradation introduced by the residual error of a Sun self-estimation algorithm described in [22]. The problem has now been reanalyzed in a wider perspective. The Sun has been directly considered in the simulations, and the aforementioned Sun self-estimation algorithm has been applied. This analysis will give insights into the effect of the residual Sun contamination after its cancellation.

Moreover, with the aim of providing a complete range of the total solar radiance, the considered Sun $T_B$ has been estimated at its minimum and maximum values, $10^5$ and $7 \cdot 10^5$ K, respectively [23], [24]. Given that the SMOS mission will likely operate during the next solar maximum, only the maximum
Sun $T_B$ results are shown, provided that the results with the minimum value do not differ significantly. Again, this analysis has been performed in both constrained and nonconstrained configurations.

It should be emphasized that Sun-contaminated pixels lie in different parts of the $10^\circ \times 10^\circ$ test area, according to the overpass. This leads to a smoothing effect when the SSS errors are temporally averaged at pixel level, which is much more noticeable in the constrained configuration. Fig. 3, for instance, emphasizes the impact of the residual Sun using the first Stokes parameter in the constrained configuration.

C. Geophysical Error Sources

With respect to the geophysical errors and misfits arising at level 3, the subsequent items address the auxiliary data impact. This impact on salinity retrieval accuracies has been studied in the past with different assumptions (for instance, in [6] and [25]). This part of the analysis, in turn, includes results from [26] and [27], but properly rearranged and tailored to be consistent with this error budget study. These studies considered the impact of multisource (models’ outputs and satellite) auxiliary data [26], [27] on the SSS error and showed a dominant influence of the wind speed as a primary sea state/roughness descriptor.

A first attempt in identifying contributions to retrieval discrepancy has been performed by splitting and isolating potential error sources with an approach which has been the forerunner of the current SSS error budget study. Two major differences can be noticed in the analysis approach between the current error budget study and these previous studies. While in the former studies the brightness temperatures were generated by Institut Francais de Recherche pour l’Exploitation de la MER (IFREMER) by forwarding a direct model, in this study, the SEPS simulator was used. This means that the $T_B$s that are available in this study are more realistic and take into account the characteristics of the instrument and the image reconstruction algorithm, which is also part of the objective of the study. On the other hand, it is important to emphasize again that, in the current analysis, only the constant input/auxiliary data have been considered in order to let the sole contribution of the parameter under study be evident in the simulations. For the same reasons, the controlled master scenario is simulated without radiometric noise.

The radiometric noise effect, which was specifically addressed in [26], has been filtered out here in order to have comparable values. Moreover, only spatio-temporally averaged ascending passes of the configurations studied have been considered. In [26], different direct-inverse models have been used, with the inverse model being the fit to the Hollinger measurements [13] used in the master scenario. This introduced a negative mean misfit in the measurements, whose nature is different from the scene-dependent bias mentioned before. Accordingly, this means that this so-called “geophysical bias” will vary according to the GMF used. To allow a comparison between [26] and the present error budget study, this effect has been removed.

Once this has been performed, the remaining effects included in such results are only the variability of the noisy reference point in the auxiliary data constraints ($SSS_{ref}$, $SST_{ref}$, and $U_{10ref}$) and the uncertainty in the auxiliary data itself (the issue under study).

The values obtained in [26] reflect the largest excursion found in the error to be related to using a different auxiliary field. Concerning the accuracy, $SST$ is capable of introducing an error of 0.026 or 0.028 psu for $Tx/Ty$ and $I$, respectively. Wind speed variation, in turn, dramatically worsens the performance of the algorithm, at least in the constrained configuration, as was already known. Depending on the external wind fields used and their difference from the original field, the results can be as bad as 0.287 psu, which is far worse than the mission requirements. It has to be stressed, however, that these numbers are related to the specific auxiliary fields considered, and even better results can be obtained by using other fields with different uncertainties. Nevertheless, this quantity is meant to provide an idea of the impact of such error on the retrieved SSS.

In the nonconstrained case, in Table II, the results in [26] have been considered again. Note that these results are the same results used in Table I, since they have been obtained in a single nonconstrained configuration. Nevertheless, neglecting constraints on salinity in this study is much more challenging, provided that SEPS quasi-realistic $T_B$s have been used.

D. Total Salinity Error Budget Assessment

The general objective of an error budget study is to provide global values which are synthetic description of the overall ensemble contributions and, in this case, whose magnitude can be directly compared with the SMOS mission requirements. Total mean misfit is the algebraic summation of the various items, while total accuracy and total rms error are the quadratic summations of the various terms studied. Three kinds of total error budgets are provided. One is related to an ideal flat sea
surface and accumulates the contribution of the radiometric errors, the Faraday rotation, and the residual Sun contamination. In turn, the two total auxiliary error budgets refer to the further contributions of these parameters, considering the degradation effect from the various SST/wind speed fields, respectively.

With regard to the constrained configuration, the total mean misfit contribution is actually rather small, while the accuracy and the total rms error are strongly affected, as expected, by the uncertainty in the wind speed. In the nonconstrained configuration, in turn, the total mean misfit is large, ranging between 0.7 and 0.8 psu. This is related to both the configuration chosen and to the level 3 weighting procedure. The latter enhances the reliability of the retrieval in the pixels with more observations and, thus, the accuracy, but to the detriment of the mean error in the final product. In this configuration, the errors induced by each item and, specifically, the residual Sun contamination are significant in the computation of the total accuracy and rms error.

V. AUXILIARY SSS VARIABILITY SENSITIVITY

In this error budget study, it has clearly emerged how the definition of the minimization setup and the tuning of the cost function can have a significant impact on the simulation results.

Since the error in the SSS auxiliary field ($\sigma_{SSS}$) is known to be a critical parameter, it is interesting to address the entire range of variability of the retrieved SSS directly related to the variability of such parameter. Indeed, this would supply direct information of the sensitivity of the SSS error to the imperfect knowledge of the reference field itself. The aim is to possibly identify whether SSS restrictions are a bottleneck for the retrieval and to ultimately establish the importance of the constraining terms.

To this end, this parameter is progressively tuned in ten different simulations starting from very restrictive conditions ($\sigma_{SSS} = 0.25$ psu) to very large values (up to 6 psu), so as to approach the conditions similar to the nonconstrained case.

Fig. 4(a) and (b) shows the graphical trends of the mean misfit, accuracy, and rms error for every step considered in this parameterization tuning. The boundary horizontal lines represent mean misfits, accuracies, and rms values without constraints in salinity.

Note two important features moving toward nonconstrained configuration: First, after an initial linear behavior, the sensitivity tends to saturate. Second, at some point, there is a crossover in the performance of mean misfit, accuracy, and rms using $Tx/Ty$ or $I$, with the latter starting to perform better.

It has to be recalled that the simulation set using $\sigma_{SSS} = 0.5$ psu is the constrained master scenario described in the first part of the study. This $\sigma_{SSS}$ value, as previously stated, has been arbitrarily chosen as a large-confidence value of the expected uncertainty on a possible auxiliary SSS field. Ideally, the actual error of an SSS auxiliary field should be used; however, this information is not yet available, and it will be derived once long time series of SMOS data are available, as has been determined in the past for the SST and wind speed fields.

In the meantime, either the standard deviation of a candidate auxiliary SSS or the uncertainty of an SSS misfit (between the “true” input and a different auxiliary field) can be used as the uncertainty of the field. Another option would be determining this uncertainty by comparing climatology or model-derived SSS fields with the ARGO-buoy salinity data (or other in situ data), even if only in specific pixels. In any case, these derived values are all well below the 0.5 psu used in the study.

Therefore, according to Fig. 4, there is a serious issue in the SSS retrieval since physically consistent values of the SSS error (around 0.25 psu, or in any case less than 0.5 psu) imply that the salinity term is overconstraining the cost function, which is undesired. On the other hand, neglecting constraints on salinity produces retrieval performances which exceed by far the SMOS requirements.

A solution could be envisaged in a proper balancing of the cost function terms by studying the gradients of each contribution to the minimization procedure. The introduction
of empirical weights could smoothen the overall influence of the SSS term while using the auxiliary fields with their corresponding physically sound uncertainties.

To summarize, the overall final products of the error budget analysis are shown in Table I with constraints on SSS, in Table II without these constraints, and in a set of simulations related only to the master scenario and its evolution as $\sigma_{SSS}$ increases. The last one would arguably provide some clues on the effective role of SSS constraints.

VI. Conclusion

This paper has summarized a number of studies carried out in the context of an SSS retrieval error budget for the SMOS payload, which is an issue that is still pending in the SMOS ocean community. Instrumental, external noise sources, and geophysical errors have been described, stressing the degree of impact on the comprehensive budget in different configurations of the cost function. In order to link these results to each other, a study concerning a tunable \textit{a priori} error on SSS has been conducted, covering different constraining regimes.

Several remarks and considerations stem from this study.

1) Salinity retrieval in the $T_x/T_y$ configuration provides better performance in both the mean misfit and accuracy than when using the first Stokes parameter in the constrained configuration. The opposite occurs when dealing with the nonconstrained minimization setting. Further attention will be paid to fully understand these trends, but they seem to be related to the different magnitudes of the background terms in the cost function in these two configurations.

2) As already known, the uncertainty in auxiliary wind speed is responsible for an important degradation of the error and is still the primary issue that will have to be addressed in postlaunch retrieval algorithm refinement.

3) For the constrained configuration, the ideal case (flat surface) error is within the 0.1-psu prescribed accuracy. Obviously, the uncertainty in the sea state/roughness that has to be included (in this case the wind speed characterization) will dramatically worsen the results.

4) Radiometric resolution implies a degradation in the error of almost the same rate for both configurations and polarizations. On the other hand, as expected, this effect is negligible in terms of the mean misfit in the selected zone.

5) Faraday rotation impact has been studied in the $T_x/T_y$ configuration, but it needs further attention, considering that it may be variable throughout the seasons and dependent on the satellite’s position. The $I$ configuration is insensitive to Faraday rotation.

6) The residual Sun contamination analysis emphasized that, despite proper correction, a large error may still be present in the nonconstrained case. An inaccurate estimation of the Sun $T_{IS}$ is not critical.

7) Salinity mean misfit (specific zone “bias”) computation indicates that, after a level 2 bias cancellation algorithm (necessary anyway due to the bias arising at level 1 using a realistic image reconstruction algorithm), some residual offset is still present and becomes large in the nonconstrained configuration.

8) The rate of mean misfit, accuracy, and rms degradation by tuning the $\sigma_{SSS}$ parameter has been studied, describing a fast initial degradation, a crossover of the retrieval performance for the two polarization cases studied, and finally a saturation effect approximately approaching the nonconstrained configuration.

9) In the constrained configuration, physically consistent SSS uncertainties may force the retrieved value to be too close to the reference prior values, thus producing spurious retrievals. This might imply that the nonconstrained configuration is adequate, but neglecting background reference information on SSS might prevent the retrieval of salinity with reasonable associated error. Future balancing of the various terms of the cost function is proposed to address this issue. Regularization factors will likely be introduced to ensure that the various terms are self-consistent.

A critical issue that still needs to be addressed to foster consensus on the inversion scheme is the assessment of a reliable GMF. After launch, during both the commissioning and the nominal operation phase, the overall salinity retrieval algorithm will surely need continuous efforts in monitoring and validating products and improving the algorithms’ performance.

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