ESTIMATE OF UNCERTAINTIES IN THE AQUARIUS SALINITY RETRIEVALS

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ABSTRACT

We present a method for formally assessing random and systematic uncertainties in the Aquarius salinity retrievals. The method is based on performing multiple retrievals by perturbing the various inputs to the retrieval algorithm. This results in calculating the sensitivity of the Aquarius salinity to these inputs. Together with an error model for the uncertainties in the input parameters it is possible to calculate the uncertainty in the retrieved SSS. It is important to distinguish between random uncertainties, which get suppressed when computing weekly or monthly averages and systematic uncertainties, which do not get suppressed by taking averages. We compare the results of the formal uncertainty estimates with uncertainty estimates based on comparing the Aquarius salinities with those from external validation sources finding excellent agreement.

Index Terms— Aquarius, Ocean Surface Salinity, Error Characterization Validation.

1. THE AQUARIUS V4.0 DATA RELEASE

The Aquarius L-band radiometer/scatterometer system is designed to provide monthly salinity maps at 150 km spatial scale at an accuracy of 0.2 psu [1]. Version 4.0 of the data product has been in released in June 2015 by the Aquarius Data Processing System ADPS.

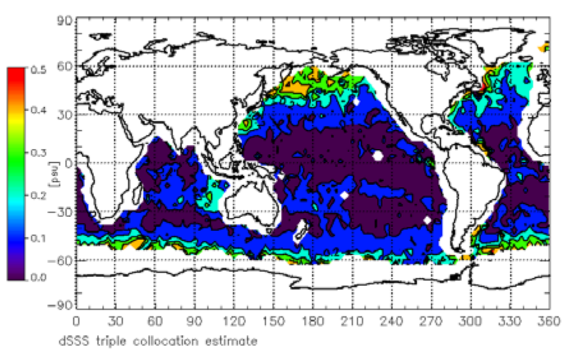

Figure 1: Estimated RMS error of Aquarius SSS over the open ocean from triple collocation analysis (SEP 2011 – AUG 2014).

The validation is based on a triple collocation analysis of salinity values that were measured by Aquarius, HYCOM and ARGO drifters. The ARGO data are taken from the monthly 3-deg gridded ADPRC field provided by the University of Hawaii (apdrc.soest.hawaii.edu). Figure 1 shows the map of estimated Aquarius SSS uncertainties over the open ocean based on the 3-year (SEP 2011 – AUG 2014) time series of triple collocations.

2. FORMAL ASSESSMENT OF UNCERTAINTIES

The basic approach to formally assess an uncertainty to the Aquarius salinity retrieval $S(x_i,\ldots)$ to a parameter x_i is to calculate the sensitivity of S to x_i. This is done by running the standard Aquarius Level 2 algorithm by perturbing its input x_{i0} by a small perturbation $\pm\Delta x_i$. The sensitivity is then computed as the derivative:

$$\frac{\partial S}{\partial x_i}(x_{i0}) \approx \frac{S(x_{i0}+\Delta x_i)-S(x_{i0}-\Delta x_i)}{2\cdot\Delta x_i} \qquad (1)$$

Assuming that we have assessed a realistic uncertainty estimate $\Delta x_i(x_{i0})$ for the parameter x_i, then the corresponding uncertainty in S is given by:

$$\Delta S_i(x_{i0}) \approx \frac{\partial S}{\partial x_i}\cdot\Delta x_i \qquad (2)$$

The assessment of the uncertainty in   consists therefore in two parts:

1. The computational/algorithm part: Running the retrieval algorithm with the perturbed parameter values.

2. Obtaining a realistic error model for all the uncertainties that are involved. This part is done offline and its results are fed into the perturbed retrievals.

3. PROPAGATION OF UNCERTAINTIES

3.1 Random and Systematic Uncertainties

We need to assign uncertainties to both the Level 2 (L2) and to the Level 3 (L3) Aquarius salinity products. The propagation of the uncertainties from the 1.44 sec measurement (L2) to the L3 averages is not straightforward, as the uncertainties have both random and systematic components. Whereas the random components are getting suppressed by a factor $1/\sqrt{N}$ when averaging over N samples, the systematic components do not but the uncertainty of the average remains simply the average of the individual uncertainties. As a consequence, it is necessary to separately assess a random uncertainty Δx_i^{ran} and a systematic uncertainty Δx_i^{sys} for each parameter x_i. This separation is not straightforward and not unambiguous. As a general guideline:

1. Uncertainties that fluctuate on larger time and spatial scales (1 month, > 100 km) are treated as systematic uncertainties.

2. Uncertainties that fluctuate on short time and length scales are treated as random uncertainties.

Every L2 salinity retrieval and every L3 map cell will contain two uncertainty values: a random uncertainty and a systematic uncertainty . The total RMS uncertainty is given by:

$$\Delta S = \sqrt{\left(\Delta S^{sys}\right)^2 + \left(\Delta S^{ran}\right)^2} \tag{3}$$

In the following we address the error propagation of both random and systematic uncertainties for the L2 retrievals and the creating the L3 maps.

3.2 Uncertainty Propagation in the Level 2 Algorithm

The retrieved salinity $S(x_i)$ depends on a number of parameters $x_i, i = 1, \ldots M$, which all have separate uncertainties $\Delta x_i, i = 1, \ldots M$. Our error model will assume that all of these uncertainties are mutually independent. However, the retrieval algorithm and the geophysical model function can introduce correlations between the different horns and polarizations. For example, radiometer noise (NEDT) is uncorrelated in all channels, whereas an uncertainty in SST results in certain correlations among the different channels.

1. Random uncertainties add in the root mean square (RMS) sense:

$$\Delta S^{ran}(\mathbf{x_0}) = \sqrt{\sum_{i=1}^{M} \left[\frac{\partial S}{\partial x_i}(\mathbf{x_0}) \cdot \Delta x_i^{ran}(\mathbf{x_0}) \right]^2} \tag{4}$$

The vector $\mathbf{x_0}$ stands for the set of unperturbed parameters $x_{i0}, i = 1, \ldots M$.

2. The conservative method for the propagation of systematic errors is to added them up straight in an absolute sense:

$$\Delta S^{sys}(\mathbf{x_0}) = \sum_{i=1}^{M} \left| \frac{\partial S}{\partial x_i}(\mathbf{x_0}) \cdot \Delta x_i^{sys}(\mathbf{x_0}) \right| \tag{5}$$

Frequently, the RMS addition (4) is also used for the propagation of systematic errors. This is based on the assumption that the various systematic errors have different signs and thus cancellation can occur in a similar ways as for random errors. For the Aquarius L2 error computation we have adopted this philosophy when computing systematic errors.

3.3 Uncertainty Propagation in Level 3 Averaging

Assuming we have $j = 1, \ldots N$ L2 salinity retrievals S_j at a certain cell with individual random errors ΔS_j^{ran}, individual systematic errors ΔS_j^{sys} and individual total RMS error $\Delta S_j = \sqrt{\left(\Delta S_j^{sys}\right)^2 + \left(\Delta S_j^{ran}\right)^2}$. We form the L3 product as weighted average:

$$\bar{S} = \frac{\sum_{j=1}^{N} \left[w_j \cdot S_j \right]}{\sum_{j=1}^{N} w_j} \tag{6}$$

with weights $w_j, j = 1, \ldots N$. The standard weighting is to set $w_j = 1$ for all j. An optimum weighting is to choose $w_j = \frac{1}{\left(\Delta S_j\right)^2}$.

The following rules apply for calculating the systematic error ΔS^{sys} and the random error ΔS^{ran} of the L3 product:

1. The systematic uncertainty of the L3 product is computed as:

$$\Delta \bar{S}^{sys} = \frac{1}{\sum_{j=1}^{N} w_j} \cdot \sum_{j=1}^{N} \left[w_j \cdot \left| \Delta S_j^{sys} \right| \right] \tag{7}$$

That means that when going from L2 to L3 we apply the conservative method (5) for propagation of systematic errors and do not allow cancellation.

2. The random uncertainty (standard deviation) of the weighted L3 average is computed as:

$$\Delta \bar{S}^{ran} = \frac{1}{\left[\sum_{j=1}^{N} w_k\right]} \cdot \sqrt{\sum_{k=1}^{N} \left[w_k \cdot \left(\Delta S_k^{ran}\right) \right]^2} \tag{8}$$

Equation (8) follows from calculating the standard deviation of the mean:

$$\Delta \bar{S}^{ran} = \sigma\left(\bar{S}\right) = \sqrt{\sum_{k=1}^{N} \left[\frac{\partial \bar{S}}{\partial S_k} \cdot \left(\Delta S_k^{ran}\right) \right]^2} \tag{9}$$

and using the expression (6). For the special case of equal random errors $\Delta S_i^{ran} = \Delta S^{ran}$, $i = 1 \ldots N$ and equal weighting $w_i = 1, i = 1, \ldots N$ equation (8) reduces to the familiar $1/\sqrt{N}$ suppression rule for the error in averages:

$$\Delta \bar{S}^{ran} = \frac{\Delta S^{ran}}{\sqrt{N}} \quad (10)$$

4. ERROR MODELS

This section discusses the major error sources of the Aquarius salinity retrieval algorithm and the quantitative assessment of their uncertainty.

4.1 NEDT

The radiometer noise (NEDT) is computed as standard deviation of the RFI filtered antenna temperatures (TF) computed over each 1.44 second cycle. This figure is then divided by the number of valid observations within that cycle that are used in the computation of the cycle average of TF. This error is treated as random.

4.2 Pointing Errors

In order to estimate the magnitude of the pointing knowledge error we compute the difference between nominal pointing (nadir) and the actual pointing that is computed from the measured S/C attitude. This value is the combination of both pointing knowledge and control errors and it thus can be regarded as an upper limit for the pointing knowledge error [4]. This error is treated as random. It turns out that its size is negligible.

4.3 Surface Wind Speed and Roughness Correction

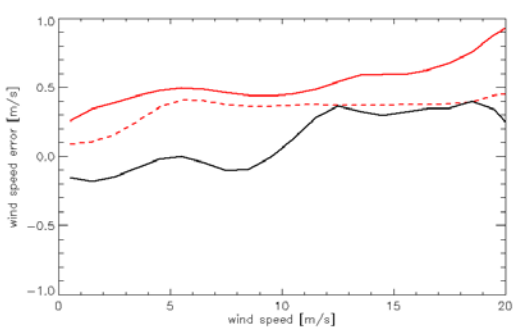

Figure 2: Estimated error of surface wind speed that is used in the Aquarius SSS retrieval: Dashed red line: Estimated random error from perturbed HHH wind speed retrieval. This curve is used as error model in the uncertainty estimation of the SSS retrievals. Full red line: random difference between Aquarius HHH and WindSat wind speed divided by $\sqrt{2}$. Black line: Estimated systematic error from Aquarius HHH – WindSat comparison.

The estimated random component (dashed red line in Figure 2) is based on running perturbed Aquarius HHH wind speed retrievals [5]. The major error sources are the noise in the L2 radiometer (NEDT) and scatterometer (Kp-value) observations and errors in the auxiliary NCEP wind speed that is used as background field.

The estimate the systematic component of this error is based computing the bias between Aquarius HHH and WindSat wind speed as function of wind speed (black line in Figure 2).

For the error in the auxiliary NCEP wind direction field we assume 10^o and treat it as random.

4.4 Auxiliary SST Input

The estimated uncertainty is the auxiliary SST input is treated as systematic. It is computed form comparing the NOAA OI SST that is used in the Aquarius V4.0 SSS retrievals with weekly SST averages from WindSat.

4.5 Non-Linear IU Coupling

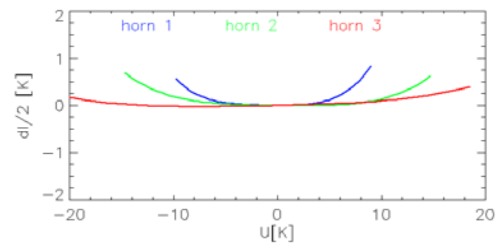

Figure 3: Estimated error in the Aquarius 1st Stokes parameter I/2 = $(T_{BV} + T_{BH})/2$ through coupling from the 3rd Stokes parameter U.

The comparison between T_B measured by Aquarius (T_{Bmeas}) and expected (T_{Bexp}), which is calculated from the geophysical model function using the HYCOM SSS field as input, reveals a significant non-linear crosstalk between 1st Stokes parameter I and 3rd Stokes parameter U (Figure 3). Because the crosstalk is non-linear, it cannot be explained by an error in the antenna patter correction (APC), which transforms antenna temperatures (T_A) into brightness temperatures (T_B) [2]. Aquarius V4.0 applies an empirical correction for this observed non0linear IU coupling. We have also included it as systematic error into our uncertainty estimate.

4.6 Reflected Galactic and Lunar Radiation

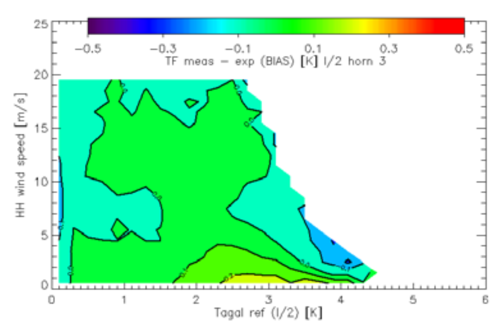

Figure 4: Bias of $T_{Ameas} - T_{Aexp}$ stratified as function of reflected galactic radiation and Aquarius HH wind speed.

The estimated uncertainty in the correction for the reflected galactic radiation are treated as systematic and based on computing the biases of $T_{Ameas} - T_{Aexp}$ and stratifying it versus the $T_{Agal,ref}$ of I/2 and Aquarius wind speed (Figure 4). Similarly, the uncertainty for the reflected lunar radiation is based on stratifying $T_{Ameas} - T_{Aexp}$ versus $T_{Amoon,ref}$.

4.7 Intruding Radiation from Land and Sea Ice

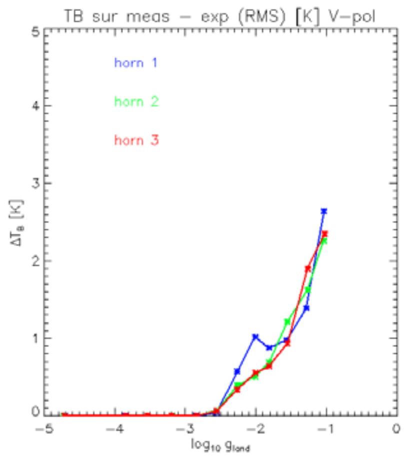

Figure 5: RMS of $T_{Bmeas} - T_{Bexp}$ stratified as function of the gain weighted land fraction g_{land}.

The estimated error due to intrusion of radiation from land and sea ice surfaces into the sidelobes of the Aquarius antenna is treated as systematic and based on computing the RMS of $T_{Bmeas} - T_{Bexp}$ and stratifying it versus the gain weighted fractions of land and sea ice within the Aquarius antenna footprint.

4.8 Undetected RFI

The error from undetected RFI can be estimated from the SSS differences between ascending and descending Aquarius swaths [6]. It is treated as systematic.

5. RESULTS

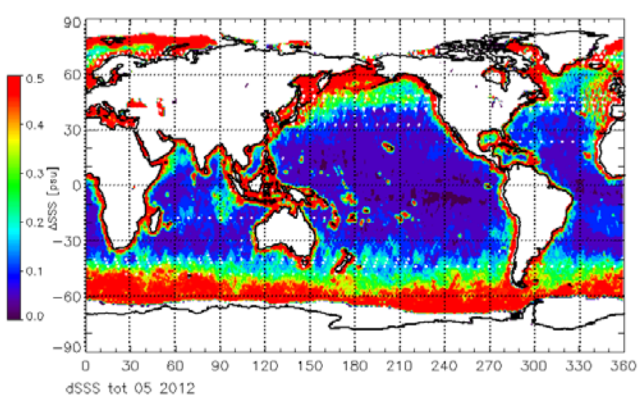

Figure 6: Total estimated RMS uncertainty of the monthly Aquarius L3 SSS for May 2012.

Figure 6 and Figure 7 show global maps for the estimated formal uncertainties of the L3Aquarius product. There is remarkable agreement between the formal result (Figure 7) and the result for the ground truth validation (Figure 1). At Level 3 most of the uncertainties are systematic (Figure 8), the largest contribution being the error in wind speed.

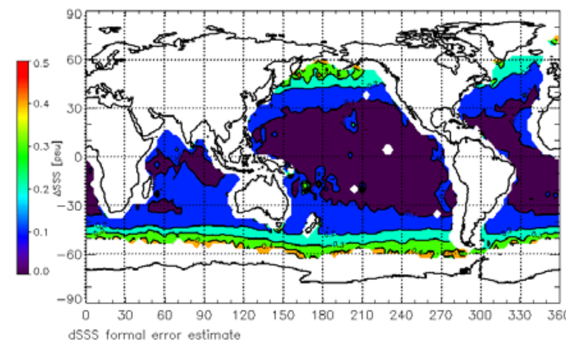

Figure 7: Estimated formal RMS uncertainty of Aquarius SSS over the open ocean (SEP 2011 – AUG 2014).

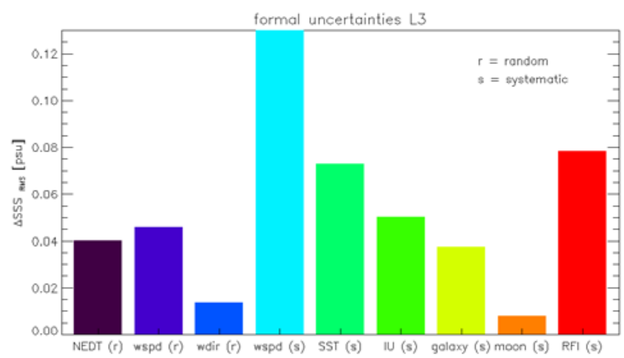

Figure 8: Contribution of the various uncertainties to the total estimated uncertainty for the monthly Aquarius L3 SSS.

6. REFERENCES

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