SMOS – Salinity Data Processing Study
WP5000 : SYNTHESIS, SUMMARY AND RECOMMENDATIONS

Nicolas Reul and Bertrand Chapron

September 2002

IFREMER

Département d'Océanographie Physique et Spatiale
Centre de Brest

Technopole de Brest-Iroise

B.P. 70 29280 Plouzané France

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1. SYNTHESIS

The MIRAS (Microwave Imaging Radiometer by Aperture Synthesis) sensor of the future SMOS (Soil Moisture and Ocean Salinity) satellite will measure microwave radiation emitted from the earth surface and surrounding environment using 72 radiometers, at frequency 1.413 GHz, in both horizontal and vertical polarisation while looking towards the earth surface at incidence angles from nadir to 55°. SMOS is designed as a 2-D interferometer. The antenna consist of 3 arms in Y-shape configuration. The polarised signals collected by the radiometers will be cross-correlated on-board in order to obtain complex-visibility functions which will be used in a pre-processing manner to reconstruct brightness temperature maps. The multi-angular viewing capability of such 2-D interferometric radiometer stems from the fact that the instantaneous field of view (FOV) is two-dimensional, extending both along and across the sub-satellite path. As the satellite moves along its track, a series of brightness temperatures emitted from the same location on the earth is observed during a short integration time for a range of different incidence angles. Spatially, the reconstructed signal is distributed along pixels with variable sizes (characteristic scale from 35 km in the center of the FOV extending to 50 km at the borders of the FOV). These resolution cells will be revisited about 10 times a month. The future L-band brightness data acquired over the ocean will be processed in order to retrieve the sea surface salinity (SSS) field. An optimal required accuracy for the future inverted SSS product is approximately 0.1 psu every 10 days over surfaces of 1°x1°, according to GODAE (Global Ocean Data Assimilation Experiment) .

From a practical point of view, inversion of the future brightness temperature signals in SSS will be possibly performed with such an accuracy if the three main following problems concerning the data processing are resolved (at least partially) during the pre-operational phases of the project:

(i) The direct problem:

Assuming a known geophysical state with given values for the main physico-chemical parameters describing the upper ocean and atmospheric system, a model is needed to correctly predict the L-band brightness temperature signal that will be measured by SMOS whatever polarisation, incidence and azimuth angles of the micro-wave emitted radiation. The direct, so-called emissivity model, should be based on solid theoretical and/or semi-empirical grounds with a well established applicability for prediction of ocean surface micro-wave emissivity. This applicability need to be verified as much as possible through experimental validation for a representative range of geophysical conditions. In particular, constraints on the ability of such model to reproduce future measurements need to be listed precisely, both in terms of the main spatio-temporal characteristics of the geophysical air-sea interfacial system, and also on the particular electromagnetic configuration of the measurement.

(ii) The inverse problem:

Given the direct emissivity model, a parametric or non-parametric adapted inversion algorithm is also needed to retrieve SSS from the future L-band brightness temperature signal measured by SMOS. An inversion algorithm is a second level development since it is based on the direct model, so that modeling errors are likely to increase with that important processing step. Consequently, the retrieval algorithm accuracy have to be well established by performing numerical, as well as in-situ retrieval experiments that take into account specific issues for SMOS. These issues include for example the effects of natural heterogeneities within the resolution cell (oceanic fronts, eddies, forcing fluxes variability) and the impact of variable pixel sizes on the retrieval processing.

(iii) The pre-operational tasks:

The pre-operational tasks concerning the data processing may be divided into three subtasks:

(1) studying the practical availability and specific character of the main ancillary data that will be needed for an accurate operational SSS inversion,

(2) Establishing the availability and requirements for natural Calibration and validation areas, and,

(3) Preparing the assimilation of the future satellite data into operational OGCM (Ocean General Circulation Models).

In this context, ESA requested a Study on Salinity Data Processing (quotation AO/1-3751/00/NL/SF, Statement of Work (SoW) APP-FP/2000-07-172/PS/ps (dated September 22, 2000) in order to advance the definition of the brightness temperature data processing for salinity retrieval from the SMOS mission. The specific objectives were :

- to advance the understanding of the physics of the interactions for the given system characteristics (L-band, range of incidence angles, dual polarization, etc.) and for several types of sea targets (cold and warm seas, rough seas, etc.);
- to assess geophysical issues specifically related to spaceborne acquisitions such as the impact of inhomogeneous surfaces (e.g. because of foam or wind variability within footprint) and of variable pixel sizes, the need for high-quality ancillary data (wind, SST) and for well-monitored sea areas to serve as references for the relative calibration of the SMOS system, by means of integrated models, finally used also to develop improved models for the simulation of brightness temperature from geophysical parameters;
- to develop algorithms to retrieve OS from the measured brightness temperatures and evaluate realistic performance targets (accuracy and spectrum of OS resolvable with SMOS data), independently of the influence of Faraday rotation.

A technical response to that request was given by a CLS/IFREMER/NERSC consortium in the present document. The study was divided in five main WorkPackages (WP) including six subtasks:

1) WP 1000 : Emission Modeling
  - WP 1100: Improvements in emissivity models
  - WP 1200: Validation using experimental data

2) WP 2000: Adapted Models and Specific OS Issues for SMOS
  - WP 2100: Heterogeneities within the resolution cell and variable pixel sizes
  - WP 2200: Availability and requirements for natural CAL/VAL areas

3) WP 3000: Retrieval Algorithms
4) WP 4000: Towards a «First Guess» Sea Surface L-Band Brightness Temperature Estimate
  - WP 4100: Data gathering
  - WP 4200: Cost-functions and refinement of the first guess Tb

5) WP 5000: Synthesis, Summary and Recommendations

The present “Synthesis, Summary and Recommendations” package (WP5000) is structured as follows: the next chapter summarizes the work performed in each four tasks, including a quick review of the problem studied for each subtask, the solution proposed and the main results; in the last chapter perspective and suggestions are proposed concerning SMOS data processing.

2 SUMMARY

2.1 WP1000 : EMISSION MODELING

2.1.1 WP 1100: Improvements in emissivity models

The problem:

The objective of this task was to improve sea-surface emissivity modeling in L-band. Various models of the electromagnetic bistatic diffusion at L-band on a rough sea surface have been used, and/or developed, during phase-A of the SMOS project. Three main types of theoretical approaches have been identified for this problem:

1) the two-scale approximation models [Yueh et al 2000, (JPL); Sobieski (UCL), 2000; Boutin et al, 2001 (LODYC);],

2) the Geometrical Optics (GO) approximation models [Camps, 2000 (UPC)],
and in the present study:

3) the Small Slope Approximation (SSA) models [Reul et Chapron, 2001 (IFREMER)].

Differences in the used/developed sea surface emissivity models for SMOS problem mainly consist in:

(i) the type of assumptions that are made concerning the rough sea surface/L-band radio waves interactions and used to resolve the electromagnetic equations,

(ii) the parameterization and semi-empirical models used to describe the sea-surface roughness within the electromagnetic models, and,

(iv) the foam emissivity modeling.

Existing direct solutions for the physics of the salinity radiometric measurement need to be studied carefully in terms of their theoretical or semi-empirical validity (applicability of each assumption), physical signification and their robustness.

Sea surface emissivity in the micro-wave band depends on the previous history of the wind and wave fields, wave age, fetch, wind variability, atmospheric stability, foam and other parameters, as well as on the electromagnetic wavelength λ and angles of observation . It is to be anticipated that in certain geophysical roughness-related situations, the emissivity models will fail to correctly predict the sea surface L-band brightness. In view of the large number of parameters involved, the best solution of the inverse problem cannot be one that relies on purely empirical relations between scattering and environmental data.

Thus, it is necessary to calculate the emissivity from a sea with a given spectrum and statistics of the rough surface. This is often accomplished using a two-scale (composite-surface) model. This model introduces a scale-dividing parameter kd separating small- and large-scale components of the roughness which can be arbitrarily chosen within wide limits. There are therefore two terms that contribute to the emission process. The first one corresponds to the Kirchhoff solution for the large-scale component (specular reflections), and the second one corresponds to the Bragg scattering solution for the small-scale component modulated by tilts of large-scale waves. This model, however, suffers from two inherent drawbacks:

1) Different authors make different choices for the parameter kd which range from k/1.5 to 40 (Wentz kd=k/1.5; Brown , Thompson kd=k/3; Durden and Vesecky kd=k/5; Jackson et al kd=k/3 to k/6; Plant kd=k/5 to kd=k/10; Donelan and Pierson kd=k/40; where $k=2\pi/\lambda$ is the electromagnetic wavenumber. The dependence of this parameter on the incidence angle and/or wind (if any) can be introduced using various guidelines. It is usually claimed that the dependence of the results on the choice of kd is weak; however, quantitative support of this statement is rarely provided.

2) Secondly, the two-scale model does not allow the evaluation of the effect of higher-order corrections on its results. Hence, the accuracy of the calculations cannot be estimated.

As a result, it remains generally unclear whether the differences between theoretical calculations and experimental data should be attributed to deficiencies of the scattering model or to the inaccurate description of sea roughness. In addition, occasionally the authors invoke modifications of the original models of the sea roughness spectrum used in their calculations ("Durden and Vesecky times 2" or "Elfouhaily's spectrum times 2"!) to achieve better correspondence between their theoretical calculations and the experimental data. The issue of consistency of the modifications with pertinent hydrodynamic data is rarely addressed. In order to take into account the loss of reflected power in a near-nadir direction due to the ripples on large waves, the local Fresnel reflection coefficient is moreover often multiplied in the Kirchhoff solution by an empirically derived coefficient close to 0.65.

Solution and results:

In this subtask we presented scattering calculations based on the small-slope approximation (SSA), which does not have the above-mentioned drawbacks. It does not invoke any arbitrary parameters. For the Gaussian statistics of roughness, the result can be expressed strictly in terms of a roughness spectrum. The SSA can be applied to an arbitrary wavelength, provided the tangent of grazing angles of incident/scattered radiation sufficiently exceeds RMS slopes of roughness. The SSA represents a regular expansion of the scattering amplitude (or the scattering cross section) in terms of the roughness slope, and both the first- and the second-order results of SSA calculations can be obtained. It can be proven that the effect of modulation of scattering by tilted facets (the basic concept of the two-scale model) is correctly taken into account by the SSA.

In our simulations we used the Kudryatsev *et al* model [34] for the sea roughness spectrum, which was recently developed based on available field and wave-tank measurements, along with physical arguments concerning the dynamics of short-gravity waves. These scales indeed represent particularly important surface components for emissivity at 1.4 GHz, since they belong to the so-called “critical phenomena” region within which surface components are dominant scatterers in L-band. It is important to note that this spectral model was developed without any relation to remote-sensing data. Moreover, by using the Kudryatsev *et al* spectral model, we avoided some deficiencies of the Elfouhaily et al spectral model as found by other (problems at the low to moderate wind speed transition).

The SSA model provides deeper insight into the physics of emission and in particular, a better understanding of the physics of the azimuthal dependence of Tb with roughness. The resonance behaviors observed in the critical phenomena region produce a significant sensitivity of emission harmonics predicted by the SSA to ocean length scales of order equal to the electromagnetic wavelength. However, these emission harmonics are also sensitive (with the exception of the fourth Stokes parameter) to anisotropy in ocean length scale much larger than the electromagnetic wavelength. A comparison between the emissivity contribution estimated from available spectral model (Apel, Elfouhaily et al, Kudryatsev et al, Durden and Vesecky) revealed that the first three model spectra would result in much larger second azimuthal harmonic predictions at low frequencies than would the Durden and Vesecky spectrum. Durden and Vesecky spectrum which unrealistically exhibits no second azimuthal harmonics for large scale waves should therefore be used with extreme care in emissivity modeling.

Azimuthal dependence as predicted by the SSA model were first compared to empirical data at higher frequencies (19 GHz and 37 GHz) than the SMOS frequency to ensure efficiency of the model. Good overall agreement with empirical data (Winrad) were found except from moderate to high wind speeds where the model generally underestimate the measured data. Effects of foam, which were not incorporated for these comparison are believed to be one of the source of discrepancy at such wind speeds and frequency. Comparison of SSA/SPM calculated brightnesses with the composite model developed at UCL, at 1.4 GHz, reveal that both model yield similar results, except in V-polarization at high incidence angles. Comparison of wind speed sensitivity with experimental data seems to indicate that SSA/SPM is more accurate in this region.

A dynamical model of foam coverage that can be directly included into a complete emissivity model was also proposed based on reported dynamical properties of breaking waves. It is expressed as function of the roughness spectrum and not solely the wind speed which ensure (i) consistency between the respective modeling of free-foam and foam-induced emissivity contributions and (ii), that sea-state development is taken into account in the whitecap coverage parameterization.

Numerical tabulation of simulated brightness temperature (Tb) data from the first-order SSA calculations (no upwind-downwind asymmetry and no foam) was finally provided for a large range of environmental conditions (SSS, SST, wind speed vector) and electromagnetic configurations (incidence and azimuthal angles and polarizations).

2.1.2 WP 1200: Validation using experimental data

The objective of this task was to validate the SSA emissivity model developed in the WP1100 as well as different submodels used in this emissivity model with WISE 2000 measurements.

During winter 2000-2001, the WInd and Salinity Experiment has been executed over an oil platform, 40 km off the Ebro river delta. A set of L band measurements were made under various meteorological conditions (wind speed from 0 to 23 m/s) with correspondent in-situ measurements made directly from the platform or from moored buoys in the vicinity. Using these different measurements, the objective was to estimate the reliability and accuracy :

- of the submodels : particularly the geometric description of the surface (wave spectrum) and foam coverage as a function of wind speed ;

- of the complete SSA emissivity model : brightness temperatures simulated by the emissivity model with measured in-situ parameters (SST, wind speed, salinity) were compared with measured brightness temperatures.

Measurements provided in the WISE 2000 packet to describe topography of the surface and foam presence do not allow validation of the submodels. The foam coverage model used in the SSA model has nevertheless be validated using UPC relation given in the Scientific analysis report (data not provided) which is in very good agreement with other empirical models.

Sensitivity of the SSA brightness temperatures to the surface wind speed for different incidence angles has been compared to the WISE measurements as well as to the Hollinger results. Sensitivities obtained with the SSA model are most of the time (H and V polarizations, incidence angles between 25 and 65 degrees) in very good agreement with the measurements and always in error bars. The weak variations of sea surface temperature and salinity during the campaign have not allowed to check the SSA sensitivity to these parameters. Nevertheless theoretical values are in agreement with expected ones.

Absolute validation of the brightness temperatures has been performed. Simulated brightness temperatures in V polarization are consistent with measurements. In H polarization, a bias of 3K appears but has to be considered carefully due to the very little amount of measurements in this polarization. For the azimutal dependence of the brightness temperatures, measurements performed during the azimutal scans have not allowed the comparison with simulations.

2.2 WP 2000: ADAPTED MODELS AND SPECIFIC OS ISSUES FOR SMOS

2.2.1 WP2100:Heterogeneities within the resolution cell and variable pixel sizes

The objective of this task was to quantify the effect of inhomogeneity in the resolution cell as well as variable pixel sizes. Originally, we wanted to test these effects in terms of impact over simulated brightness temperatures. As we had already processed an inversion algorithm (see

WP3000) when we began this task, we decided to test these effects directly in terms of error on salinity retrieval. To make a realistic evaluation of these effects, we needed a realistic description of the surface with a very good spatial resolution.

The Suroit measurements from the Catch/Fastex experiment have therefore been used to test some particularities of SMOS pixel with realistic variations of the sea surface parameters.
In-situ measurements used for this study were presented in detail. Two specific issues for SMOS were studied: the first one consists in the inhomogeneity of the sea surface parameters in the SMOS pixel and the second one in the fact that the different brightness temperatures used for the salinity retrieval correspond to different pixel sizes. The impact of correlated errors in ancillary data was also studied since these errors will increase the error estimates on SSS retrieval compared to the error calculated with the assumption of independence of the data. The correlation of the errors for the wind was examined using two different wind sources.

Impact of inhomogeneity of the sea surface:

The impact of inhomogeneity of the sea surface in the SMOS pixel has been tested in two particular situations:

1) The first one is a case of a strong SSS/SST front. Individual retrievals for each subcell were found very satisfactory. The retrieval from the average brightness temperatures without noise presents a bias of 0.2 PSU with the reference value. The values obtained from noisy brightness temperatures were even more underestimated (-0.36 PSU). For such a situation (1.5 PSU variation), these results were found acceptable.

2) The second case was a situation of very strong wind speed gradients (between 9 and 29 m/s in the pixel). The individual retrievals were satisfactory everywhere except for the very strong wind speed value (29 m/s), which was not present in the database. This is why the modification of the brightness temperatures by the surface roughness in this case was misinterpreted as a salinity modification. The retrieval from average brightness temperatures was correct in the case of no noise but an unacceptable bias of -1.75 PSU appears when a realistic noise was added to the brightness temperatures. In this situation of very strong wind

speed, the effect of adding a noise leads the algorithm in a domain where it has not learned. This result is not so critical since 1) this result does not give only the influence of the heterogeneity but includes also the error in the retrieval processing, 2) very high wind speed values are missing in the database.

Impact of the variable pixel sizes:

The impact of the variable pixel sizes has been estimated using the SSS/SST front situation, and three different positions of the front in the largest SMOS pixel (50kmx50km):

1) In the first case the pixel is chosen located at nadir. All brightness temperatures were noise-contaminated in this case, but the important variations between the parameters used for the different incidences makes the retrieval difficult. Results obtained with or without noise showed important differences with the nadir value (0.5 and 0.8 PSU).

2) In the second case, the front was located at 40 km from the subsatellite point (only 40, 50 and 60° brightness temperatures were contaminated). Results obtained with or without noise were found satisfactory (0.1 and 0.2 PSU of difference). In the first case all brightness temperatures were contaminated by the front but the difference in SSS and SST between the different surfaces was very important (0.59 PSU salinity amplitude variation). With the second case, only 3 surfaces were contaminated but the variation of the salinity was weaker (0.2 PSU). This explains the better results.

3) The last case corresponded to the front located at 55 km from the subsatellite point (the front is only present in the 60° pixel). Using brightness temperatures without noise gave a bad result (difference of 0.5 PSU). This shows the impact of the 60° brightness temperatures in the retrieval. Adding noise to average brightness temperatures gives better results. This can be explained by the fact that *algorithm 2* (see WP3000) has learned over noisy brightness temperatures and that this noise can be interpreted in this case as a modification of the geophysical parameter for one incidence angle.

Impact of error correlation:

As a conclusion for the "errors correlation part", the ancillary data error in wind and SST within the GODAE averaging (200kmx200kmx10days) cannot be assumed independent. From crude estimates, the wind error of the mean is globally of 0.5 m/sec which leads to an error on brightness temperature of 0.1 K under the assumptions of no foam and incidence angles lower than 40°. The SST error of the mean in the Atlantic Ocean is of the order of 0.4°C. To quantify these errors in term of error on the SSS is not straightforward since no simple relation exists between wind, SST and retrieved SSS. These numbers are to be used with caution and for gross estimation only, since many assumptions are made, and the error on wind or SST calculated from the difference of two fields from different sources is not a robust method. However, we proposed herein a method for error estimation, using the fact that errors are not independent.

2.2.2 WP 2200: Availability and requirements for natural CAL/VAL areas

In this task, four types of calibration for the SMOS brightness temperatures have been identified.

1) The first method we propose is the one used for the calibration and survey of the ERS2 and Envisat radiometers. It consists in the regular comparison between measured and simulated brightness temperatures. Simulations are performed over model grid with estimation of the different geophysical parameters needed in the radiative transfer model for the computation of the brightness temperatures. Satellite measurements in spatial and temporal coincidence with model outputs are extract. The statistical comparison between measurements and simulations are then analyzed in details. The main advantage of this method is to perform a calibration consistent with the retrieval algorithm. This is the case if the model and the radiative transfer model used for the calibration are the same than those used for the algorithm formulation.

2) The second one consist in the calibration using ocean brightness temperatures. For the Topex radiometer in-flight calibration, C. Ruf has developed a method using the lower brightness temperatures over ocean. The survey of the colder part of the TBs histograms makes it possible to detect very weak drift. We have shown that in case of SMOS, this colder points will mainly come from salted and cold waters. Furthermore these high latitudes situations seem very favorable with weak atmosphere contribution, weak ionospheric activity, low sensitivity of the TBs to the salinity in cold waters. Ocean parameters driving brightness temperatures in L band are sea surface salinity, temperature and wind speed. Using WOA98 database we have identified stable (spatially and temporally) areas in terms of salinity and temperature. Adding a criteria of wind speed variability should make possible the identification of ocean stable areas.

3) The third calibration can be performed over hot and cold continental targets. The cold targets identified here are the Dome C of Antarctica, and two little areas over the Antarctica Plateau and Greenland Glacier. These areas are quite stable in time and temperature, and the annual cycle can be removed. The hot targets are the Sahara Desert and the Amazonian Forest. The Sahara desert is used for the TMR and ERS2/MWR survey but due to the important penetration in L band, rocks deserts like Australian desert should be maybe more appropriate. The part of the Amazonian Forest that we selected is very interesting since it can be considered as a black body (emissivity of 1, independent of the frequency and polarization). Nevertheless this assumption has to be confirmed in L band.

4) The last possibility is to use the sky as a calibration target. In their paper, Delahaye et al have identified a part of the sky corresponding to the Celeste North where the brightness temperature is minimum and where the calibration will be always possible.

All the calibration methods presented here have to be reconsidered in the context of the SMOS calibration. They are used routinely for the survey of the different channels of in-flight radiometers. All these channels differ by their frequency but have the same viewing angle. The analysis of measured brightness temperatures at different frequencies will become a multi-angle analyze in case of SMOS. In this case, it will be necessary to know what type of problems may occur, and what brightness temperatures may be affected.

Frequencies for classical radiometers referred in this document are quite similar. This is why, often the difference between 2 channels is used to remove the natural variations of the brightness temperatures. How should be analyzed the difference between 2 different incidence angles SMOS measurements, or between 2 different polarization to get similar conclusions ?

Continental areas suggested here are currently used for the calibration of radiometers at frequencies higher than 10 GHz. But it is necessary to assess the feasibility of using the same areas for the SMOS calibration. In sand, forest, ice, the penetration in L band will be stronger and it appears necessary to get an idea of the signal of such areas in L band using surface emissivity models and /or in-situ measurements.

2.3 WP 3000: RETRIEVAL ALGORITHMS

The objective of this study was to investigate several inversion techniques and develop algorithms to retrieve salinity from the SMOS measured brightness temperatures.

Two approaches have been compared : neural network and classical linear regression algorithms. The neural network method has been selected and was analyzed in depth in this report.

The use of neural network method for salinity retrieval is totally justified when comparing the results with a classical linear regression. The neural network algorithm better retrieves non linear dependence between salinity and brightness temperatures.

Whatever the method used, one key point for retrieval is the constitution of a *representative database*. A lot of work has been done to build a database with enough data and where many different situations as possible are represented.

Certainly, this database can be improved by adding more extreme situations for the salinity and also more different combinations of (SSS,SST,U).

This study shows that the noise level expected on the brightness temperatures for SMOS clearly alters the quality of the salinity retrieval. Nevertheless, performances obtained in the case of realistic noise remain satisfactory. Similarly, the test made with a bias on brightness temperatures proves that the retrieval is very sensitive and that the bias will be a critical issue (a small value of 0.5K provides an error of 1 psu on salinity). Above all, it induces variations of salinity which are not reduced to a simple bias, and this will make it very difficult to correct this effect, using in-situ measurements.

The influence of the ancillary parameters is of importance for the salinity retrieval. It does help the retrieval to converge towards a better solution. When adding a priori sea surface temperature and wind speed, the dispersion is reduced. A first guess salinity allows better regression for extreme values of salinity. The error on salinity is of 0.51 psu in a realistic configuration for SMOS sub satellite track. This value is a mean error computed globally, for all the different situations. The error on salinity, in some areas like the high latitude region will be surely more important. All the results presented in this report show that low values of salinity are always difficult to retrieve. It is explained by the weak sensitivity of the brightness temperatures to the salinity for cold waters, generally associated to low salinity values. One point to improve retrieval performance would be to better assess the situations of low salinity and temperature.

The validation of the retrieval algorithm with WISE measurements has not been performed. Since the WISE measurements provide very few H polarisation brightness temperatures and only for some incidences, the proposed algorithm for the subsatellite track using 7 incidences and both polarisation can not be applied. In accordance with ESA, this task was replaced by the study of inversion algorithm with the sum of H and V polarisation, which presents greater interest.

The Faraday effect has been tested and it appears it can hugely affect the retrieval. One way of solving this problem is to tune a retrieval algorithm with the sum of H and V polarisation. The error on salinity when using only the first Stockes parameter is of the same order as the error obtained when using separate polarisation. Thus, this configuration is recommended and the annex gives the specification for this algorithm.

2.4 WP 4000: TOWARDS A FIRST-GUESS BRIGHTNESS TEMPERATURE ESTIMATE

2.4.1 WP 4100: Data Gathering

In WP4100, we reviewed how satellite sensors and models may be used to determine the most important ancillary parameters for SMOS and we described the main problems associated with the collect of these data. Major conclusions are the following:

1) ***For SST***:

It will be crucial to merge the SST data obtained from microwave and IR sensors in order to solve problems associated with the presence of cloud cover and the diurnal SST cycle. Spatial and temporal resolutions of SST sensors are in general higher or equal to the future SMOS measurement resolution: therefore, their resolution should not be sources of problems to generate a co-localized SST gridded-data with SMOS measurements (spatial resolution around 35 km every 6 hours).

2) ***For roughness***:

2.1 Wind vector:

Scatterometer and radiometer observations over the ocean provide direct estimates of the global wind vector field at spatial resolution less than or equal to O(50km), with an accuracy of ±1-2 m/s in speed, 15° in direction, but usually with a directional ambiguity of 180°. To get an a priori information on the wind heterogeneity and for SMOS measurements in semi-enclosed seas, in straits, in coastal regions, and in estuaries, scatterometers and radiometer resolutions (> 25 km) will be however too coarse. In these cases, one can use wind field estimates retrieved from high-resolution SAR images with a spatial resolution of typical 10 x 10 km, when available and numerical weather prediction models (ECMWF, NCEP). To solve the temporal resolution problem it is suggested to use merged QuikSCAT and ADEOS-2 wind vector data. Recently, blended products have also been regularly produced (http://dss.ucar.edu/datasets/ds744.4/data/) to attenable brute force merging between model and satellite inputs.

2.2 Other sources of roughness information:

Sea surface emissivity in the micro-wave band depends on the previous history of the wind and wave fields, wave age and fetch. Therefore wind vector is a necessary but not sufficient parameter to describe roughness. Significant wave height (Hs) could be determined using satellite altimeter measurements, swell direction and wavelength will be possibly determined using SAR or numerical Wave prediction models.

3) *For Surface Salinity:*

A priori knowledge of the surface salinity will be necessary for calibration of the instrument but also because errors on the retrieved brightness temperature will be reduced if a first guess surface salinity can be provided (See WP 3000). Moreover, the measured surface salinity from SMOS will have to be physically coherent with the underlying circulation dynamic in the ocean upper-layers, and especially, coherent with vertical and horizontal known distributions of salinity as predicted by numerical model of ocean circulation. This is fundamental in the perspective of the future surface salinity data assimilation within ocean models. This coherency could be achieve by association, comparison and correction of measured surface data with model data, given by ORCA, NANSEN or CLIPPER circulation models.

Lastly, we briefly review potential techniques to merge satellite and model data on a co-localized grid with SMOS measurements. We recommend the use of the Krieging method which is based on an objective analysis for merging all available sources of information concerning each ancillary parameter that play a key role in SMOS SSS retrieval.

2.4.2 WP 4200: Cost functions and refinement of the first-guess Tb

In this subtask, we have considered several experiments where simulated Tb data were assimilated into an OGCM (HYCOM) using the Ensemble Kalman Filter which is currently used to assimilate SST, SLA and ocean color data. Five experiments were designed assuming the following instrumental settings:

Angle of incidence=40.0°;
Azimuth angle=0.0° ;
Wind=0.0 m/s;
Polarisation=vertical,
Variance in observations equal to 0.0025 $°K^2$ (Case 1-4) and 0.25 $°K^2$ (Case 5)

Various synthetic Tb data sets were created using the modelled SSS and SST. Different variants of the TB data sets were created, e.g., by adding random perturbations to the synthetic data and by setting either SST or SSS equal to a constant. This allowed us to give a first assessment of the impact on the model state of assimilating Tb data. We focussed the attention on the effect on the SST and SSS variables.
This resulted in the following major findings:

-The assimilation of the Tb data proved efficient for controlling the model SSS and to some extent also the SST.

-The assimilation of the Tb data less impact at high latitudes than at mid latitudes. This was most likely an effect of typically lower variability in the model prediction at high latitudes compared with mid and low latitudes. Further studies are needed to better understand this issue.

-Future satellite observed Tb data are likely to serve as an important source of information in operational ocean data assimilation systems, provided that the data can be delivered with sufficient accuracy and resolution.

3 PERSPECTIVES AND RECOMANDATIONS

3.1 EMISSIVITY MODELING:

3.1.1 Improvement in emissivity modeling:

If one take also foam effects into account, the main submodels of a complete emissivity model for the sea surface in L-band are :
_ the dielectric constant model at 1.4 GHz ,
_ the electromagnetic model (SSA, two-scale,…),
_ the spectral model of surface roughness W or/and the surface slope distribution function,
_ the foam coverage model F, and,
_ the emissivity model ef for foam.

Submodels used in the present model are the Klein and Swift model for ε, the semi-empirical Kudryavtsev et al, [1999] spectral model for W and specific models have been developed for F and e_f (Reul and Chapron 2002, contrat ESA n°14273/00). The main weaknesses and limits of the present complete emissivity model are the following:

1) in theory, it should only be valid for surfaces where roughness elements (waves) have small slopes. This condition is a priori verified on average at the ocean surface but locally surface slopes might be large, particularly during storms events. These effects are not yet taken into account. We suggested to use a similar approach than the one proposed by Voronovich et al. for active scattering modeling to account for large slopes, e.g., to use a Geometrical Optic scattering model applied to a probability distribution function for high slopes.

2) while being a priori the most adapted model for □, Klein and Swift model have been only partially validated at 1.4 GHz. New experimental measurements of □dependence with SSS and SST at L-band have just been performed by S. Blanch and A. Aguasca. The SSA model should be therefore run again with this new, more confident, empirical dielectric constant model.

3) the spectral model used to describe sea surface represents a sea state at statistical equilibrium. Consequently, it doesn't take into account presence of swell, current and unsteady growing or decaying sea states.

4) theoretical developments performed to predict upwind-downwind asymmetry in the brightness temperature are based on assumptions that still need to be verified (reduced bispectra) and compared to empirical measurements.

5) models developed to evaluate foam contribution to L-band emissivity are dependent upon a large number of parameters with exact values and variability difficult to quantify.

6) while the current SSA code is simpler to implement numerically than traditional emissivity models (a double integral is replaced by a single one), it was not optimized in term of CPU-time. An effort is needed to achieve a faster computation time.

Therefore, we recommend that a research effort should be carried on to include in the SSA model the effects of frequently encountered phenomena at the surface of the open ocean like swell, high (large slopes) and low (surfactant effects) wind stresses.

3.1.2 VALIDATION USING EXPERIMENTAL DATA:

Measurements provided in the WISE 2000 packet to describe topography of the sea surface and foam presence do not allow validation of the emissivity submodels (except for foam coverage). New results from the very recently performed WISE 2001 and Eurostarrs campaign should be used to improve the validation of the SSA models. These campaigns indeed provide brightness temperature data with increasing accuracy and statistics. However, it is believed that a larger effort should be carried on to precisely measure roughness characteristics concomitantly with radiometric measurements. This point is crucial to correctly determine whether the emissivity model or the surface descriptor do fail or have success to simulate reality. Wind vector is a needed parameter but it is not sufficient to describe precisely roughness. Systems to measure precisely sea surface roughness directional spectrum over a wide range of surface scales can be divided into two parts: in-situ direct measurements and remote measurements. Wave rider buoys were often used in the past to validate active measurements. The ASIS (Air Sea Interaction Spar) buoy developed at the university of Miami by M. Donelan (see http://anole.rsmas.miami.edu/people/mdonelan.html) is equipped for high resolution wave directional measurements, as well as atmospheric surface layer structure. It might be a very good tool to help validating emissivity models in the open ocean, as it was the case for active models validation (SHOWEX, SEMAPHORE, FETCH campaigns …). The second type of roughness measurements include optical devices (Riegl laser altimeters used in an integrated airborne or ship measurement system for the determination of surface wave field properties, see Crescenti et al. 1999 during SHOWEX) or active microwave sensors (scatterometers). It is believed that one of these three techniques should be used in a future SMOS pre-validation campaign. At L-band, GPS-like measurements should as well be promoted as already studied under ESA/OPSCAT studies.

3.2 RETRIEVAL ALGORITHM:

A first SSS inversion algorithm based on a direct emissivity model in L-band has been proposed in this study using a neural-network technique. The following points have been concluded :

1) a key step is to constitute a representative data base to train the network using realistic SST, SSS and wind data fields,
2) the radiometric noise has a strong influence on the accuracy of the retrieved SSS, and,
3) the use of ancillary data (SST, U and a first guess SSS) as input data in the network significantly improve the accuracy of the retrieval.

Perspective to improve processing steps 1) and 3) are the following :

1) To build an adapted algorithm for ranges of SST values:

In the present study, the SST and SSS data used to construct the neural network has been extracted from the WOA97 World Ocean Atlas. Quickscat-scatterometer products have been used for the wind data. In the range of incidence angles used by the SMOS sensor, the brightness temperature (Tb) dependence with wind speed is quasi-linear and this parameter doesn’t influence in a critical manner the retrieval accuracy. The sensitivity of Tb with SSS and SST is however strongly non-linear in that range. For typical SSS values in the open ocean, $\delta Tb/\delta SSS$ indeed gets smaller as SST gets lower. As the neural network algorithm was constructed using a global data base, the weight of low SST values, and therefore low SSS sensitivity, induce a global loss of accuracy in the retrieval.

The proposed approach would consist in selecting adapted data basis from the global data base by classes of SST values (these classes could be selected as function of the sign of δTb/δSST). Individual neural network algorithms would then be trained using each individual SST-driven data base, and finally patch together to obtain a global inversion algorithm. It is believed that the global inversion algorithm should be therefore more accurate at low SST values.

2) To use a first guess SSS value from radiometric measurements at nadir:

Numerical simulations performed on the neural network algorithm revealed that a first guess SSS value at the time and location of SMOS measurements would significantly improve the retrieval accuracy. This first guess SSS could be given from numerical Ocean General Circulation Models outputs. However, in view of the future use of SMOS-retrieved SSS values for assimilation in OGCM, it would be much better to get that first guess SSS value from a model-independent source. The idea is to use the peculiarities of the polarized brightness temperature signals measured at nadir.

In a joined document entitled "*A simple algorithm for Sea Surface Salinity retrieval from L-band radiometric measurements at nadir*", we show that an enhanced inversion accuracy could be *a priori* reached using the properties of the polarized signals emitted by the sea surface at nadir. This enhanced accuracy is expected since (1) a simple inversion algorithm can be analytically provided at normal incidence and (ii) the inversion solely demands knowledge of two ancillary data: locally-averaged SST and wind direction, so that the solution is no more wind speed dependent. For further details, see the joined document.

Solution of this first-level algorithm should help to directly inverse SMOS measurements in a simple manner to get first-guess SSS values without *a priori* knowledge of the wind speed but only its direction. Using these first-guess SSS values as input to the neural network would then allow to combine nadir and non-nadir measurements to improve SSS retrieval. Such simple algorithm was the basic idea of the SKYLAB salinity measurement project. We must also recall that such a method was promoted by C. Swift to approach the problem. The satellite mission project was not selected for lack of spatial resolution but the methodology can be pursued for SMOS. AQUARIUS satellite sensor will not have the ability to deal with measurements at nadir and it is believed that SMOS configuration at nadir represents a great potential that we shall explore. Combining H- and V-pol is moreover very promising since Faraday effects are greatly reduced when summing both signals.

It is therefore suggested to study the potentiality of such algorithm:

- by first carrying dedicated studies using available radiometric data at nadir and in frequency bands close to L-band (e.g, S-band measurements by Y. Trokhimovski),

-by performing an airborne campaign where an L-band radiometer would be operated at nadir in both H and V polarization together with an SST measurement and in-situ SSS measurements.

3.3 SPECIFIC ISSUES FOR SMOS:

Concerning specific issues for SMOS,

3.3.1 Defining the « skin-salinity » :

The surface skin-layer depth δp (depth at which electromagnetic waves do penetrate sea water) depends on the electromagnetic frequency, the salinity and the temperature as it is function of the dielectric constant. The question is to know if we can define the future salinity measured by SMOS satellite as a coherent parameter for oceanographers, since the satellite will measure a skin-salinity in analogy with the skin temperature measured by infra-red radiometers [Saunders, 1967; Katsaros, 1980; Stewart, 1985]. Empirical coefficients which are used in inversion algorithm to get SST values from radiometric measurements are actually calculated using regression laws applied to *in situ* data. Buoy networks and drifting sensors therefore play a major role for remote sensing of SST. Similarly, it is to be anticipated that future SSS data from SMOS will be routinely calibrated from *in situ* measurements as well. Knowing that opportunity ships, buoy and drifting sensors (PROVOR/PALACE) are sampling salinity up to 3-5 meters underneath the air-sea interface, it is important to anticipate the variation of salinity in the first centimetres of the surface layer.

For low SSS values, $\delta p < 1$ cm at 1.4 GHz and the skin effects should not be significant in such thin layer. However, for the majority of encountered SSS values in the open ocean, $1<\delta p<5$ cm and skin effects might be important especially for low wind speeds and high precipitation rate (particularly in tropical areas). Physical mechanisms that might generate strong salinity gradients in the first few centimeters underneath the surface are mainly evaporation and precipitation. Saunders (1967) proposed a model of the change Δc of the salt concentration due to evaporation only. He estimated that $\Delta c/c$ can reach a maximum value of approximately 2% in presence of large variation of specific humidity. If the wind is moderate or strong, the turbulent mixing-layer spread down to few meters underneath the interface; if the wind is weak, we expect a maximum evaporation at day time of approximately 0.1-0.2 cm which corresponds for a 1 m deep surface-layer to a change of approximately 0.03 to 0.05 psu in salinity. Effects of precipitation are to reduce the surface salinity and to decrease density, which have a stabilizing effect on the density gradient. If winds are low, the mixing of surface layers is also weak and the fresh surface layer can persist for a certain time. To our knowledge, no model is yet available to evaluate surface salinity gradients due to precipitations and Saunders (1967)'s model for evaporation effects has not yet been experimentally validated.

Although the recent measurements conducted during the WISE2001 campaign revealed that there were no significative differences between 5 meters depth and surface salinity measurements, we stress the importance of correctly evaluating the skin-salinity effect for tropical areas where SMOS measurements should be the more accurate (due to measurement sensitivity at high SST) and were low wind and high precipitation conditions are frequently encountered.

3.3.2 Heterogeneities within pixels:

The first perspective that can be given to this part, is also an improvement in the building of the database used for the tuning of the retrieval algorithm. The impact of the inhomogeneity in the pixel could be reduced adding other situations of wind speed for a given SSS and SST in the database, particularly strong values of wind speed. The important effects of the variable pixel sizes that we observe on salinity retrieval are mainly due to the fact that the algorithm has learned over 13 brightness temperatures generated from exactly the same set of geophysical parameters. If we try to inverse brightness temperatures corresponding to different situations (even if differences are weak), the retrieval is difficult. One way to avoid this effect is to complete the database. For a given set of (SSS, SST, U), it is possible to generate 7 different sets (one per incidence angles) of noisy parameters with an appropriate distribution and to compute the brightness temperatures from these parameters.

Concerning the errors correlation, there is a need to better assess the consequences of such correlations in salinity retrieval. The SMOS End to end Performance Simulator (SEPS) would be a valuable tool to quantify this impact in simulating a realistic space/time averaging. It would be interesting to introduce the correlation field of errors on ancillary data, and verify how it modifies the reconstructed salinity field.

3.3.3 CAL/VAL areas

The selection of dedicated areas to the SMOS calibration requires a quantitative estimation of the emissivity of the potential surfaces (particularly concerning continental targets). And this will be possible using either in-situ measurements in L band when available over this type of area or accurate models to simulate their emissivity.

3.4 SMOS DATA PRE-PROCESSING STEPS:

3.4.1 Data gathering: Merging active and passive sensors to estimate roughness

Except at nadir incidence angle, the roughness contribution to the brightness temperature ΔT_b cannot be removed. Due to the high sensitivity of brightness temperature measurements to surface roughness, it is crucial to correctly estimate the latter at SMOS pixels. The radar cross sections σ_o and the brightness temperatures T_b that are respectively measured by scatterometers, altimeters, SAR, and radiometers, are physically more correlated with the ocean surface roughness and friction velocity than with the wind speed which is extracted from these signals. It seems therefore more interesting to directly correlate the future SMOS measurements with σ_o and T_b, as measured by other sensors. Indeed, if we assume (i) Bragg scattering to be the dominant scattering mechanism at the sea surface and (ii) that surface scattered signals are characterized by a small upwind-downwind asymmetry, both the roughness contribution ΔT_b to the brightness temperature and the radar cross section σ_o are proportional to the sea surface spectrum. Consequently, if two sensors, one active and the other passive, are probing the sea surface at electromagnetic frequencies f_1 and f_2 close to each other, it is reasonable to expect the following quasi-linear relationship:

$$\Delta T_b(f_1) \cong a\,\sigma_o(f_2) \qquad (1)$$

where *a* is a proportionality factor (Yueh et al, 2001). This simplified linear model suggests that radar cross-section measurements could be used to correct roughness effects on the future SMOS brightness temperature measurements. This is indeed the central idea for the future AQUARIUS scatterometer concept. It is suggested here that the same approach might be powerful to remove roughness effect for SMOS, if active measurements are provided at a frequency close to L-band and with small spatio-temporal delays with regard to SMOS acquisitions.

Good candidate for such application might be of course the future AQUARIUS scatterometer (1.2 GHz) but also the GPS L-band reflected signals. Since the GPS reflected signal technology may not be operational during SMOS mission, a study should be carried on to estimate the acceptable frequency difference $\Delta f=(f_1-f_2)$ between SMOS radiometer and potentially available active sensors for the quasi-linear relationship above to stay valid. This should help to identify which available active sensor to use. A study should be therefore dedicated to estimate how large Δf can be for Eq. (3) to stay valid as function of available active sensors operating at frequency f_2.

3.4.2 Data Assimilation:

Concerning assimilation of Tb in OGCM, the impact of using different polarizations, incidence angles and wind speeds have not been examined in the present study. This work must be characterized as a first preliminary study where we demonstrate a capability and a positive impact of assimilating Tb data into an ocean model. Future work will require more elaborate sensitivity studies where Tb data are generated using different parameter settings, and it will also be important to examine the impact of assimilating Tb data together with data from other sensors, e.g., SLA and SST data.