Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring:

Deliverable 4.7: Report detailing approach to the calibration and validation of (atmospheric state variable) EO data, and detailing proposed approach to other ECVs and associated EO data

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1. Introduction

The aim of Work Package 4 (WP4) of the GAIA-CLIM project was to assess and develop the capability of global Numerical Weather Prediction (NWP) systems to contribute to the validation of new satellite observations. Work Package 4 focussed on microwave radiance observations from satellites and the scope was limited to observations with primary sensitivities to atmospheric temperature and humidity. It has been shown, as part of WP4, that global NWP systems are able to identify and characterise a range of biases in satellite-radiance measurements. This has been illustrated though an assessment and analysis of data quality from a range of satellite sensors, including those from Chinese, Japanese, Russian and US satellite agencies. Furthermore, WP4 has shown how reference quality measurements from the Global Climate Observing System (GCOS) Reference Upper Air Network (GRUAN, Dirksen et al, 2014) can be used to sample and characterise biases in NWP models themselves and thereby help define the uncertainty characteristics of the models. The aim of this report is to assess to what extent the methods developed in WP4 *generalise* to a wider set of Essential Climate Variables (ECVs). This report forms Deliverable D4.7 for the GAIA-CLIM project.

In considering the generalisation of the approach to a wider set of ECVs it is worthwhile noting the key features of NWP systems and supporting systems that enable them to be exploited effectively for satellite validation:

- **A comprehensive observing system**. Current NWP systems make use of a diverse range of observations, including conventional in-situ measurements at the surface and the upper atmosphere, as well as from a constellation of satellites operating in geostationary and low Earth orbits. The capabilities of this observing system, in terms of spatial coverage, temporal continuity and accuracy, have been improving steadily since 1979. This has resulted in a degree of spatial homogeneity in the quality of the model fields, at least for some parts of the atmosphere. Plans are well developed to continue the coverage provided by key datasets (satellite radiances, for example) for the next three decades and beyond. There is, therefore, a high likelihood that the capabilities for satellite validation provided by NWP systems will be *sustained* for the longer term.

- **Sophisticated data assimilation systems**. Data assimilation systems are designed to provide accurate analyses that serve as initial conditions for NWP forecast model runs. In atmospheric reanalysis mode (Dee *et al*, 2011, 2014) the same systems are used to generate consistent analyses of the global atmospheric state over decadal timescales. In NWP, such systems have evolved as a result of concerted and sustained research and development effort since the 1980s. These systems aim to optimally blend new observational information from the observing network with *prior* information on the global atmospheric state, normally in the form of a short-range forecast from a previous analysis. The relative influence of the observational information and the prior information is determined by the error characteristics of both. In current state-of-the-art systems, the use of a forecast model to consistently interpret observational information throughout the analysis window (typically 6-12 hours long) ensures the resulting analyses are physically balanced.

- **The development of reference observation networks.** In recent years, the importance of establishing networks of high quality reference measurements has been recognised. These reference observations are characterised by an aim to achieve the highest possible accuracies, enabled though establishing metrological traceability to recognised measurement standards.

The GRUAN network was established to provide high-quality observations to support climate trend analyses (Seidel *et al*, 2009), to calibrate and validate data from more spatially comprehensive observing networks (including satellite data), as well as to support process studies. In the approach developed in WP4, the role of these reference observations is to *sample*, and *characterise*, the error characteristics of the global NWP models, in terms of both temperature and humidity, but also their top-of-atmosphere brightness temperature equivalents.

The particular strengths of the global (NWP) analysis-based approach to satellite validation can be summarised as:

High sensitivity. As the NWP system makes near-optimal use of the comprehensive observational information available, the resulting model equivalents of new observations can be used to identify and characterise biases in satellite observations with high sensitivity. Based on experience gained as part of GAIA-CLIM, these can be estimated to be: around 0.1K for tropospheric temperature sounding channels; 1.0K for humidity sounding channels; and 2-5K for surface sensitive channels.

Global coverage. The global NWP models provides complete global spatial coverage, at spatial resolutions of 10 - 50km. This has proven to be particularly valuable in characterising biases which are exhibited over short spatial scales or exhibit complex spatial structure over large areas, and in elucidating the mechanisms causing these biases.

Continuous temporal coverage. The NWP systems run continuously and therefore provide unbroken time series of statistics on aspects of satellite performance. This has proven to be very valuable in identifying transient biases in satellite data and in identifying the precise time of sudden changes in satellite-data quality.

One area of weakness in the NWP approach is the ability to determine the absolute biases in satellite observations. This has been tackled in GAIA-CLIM WP4 through the use of the GRUAN reference observations.

This report aims to assess, for a wider set of ECVs than those examined in WP4, which of the building blocks are in place to allow global analysis systems to be used effectively for the validation of new satellite observations, and what are the future prospects. The scope of the assessment has been limited to ECVs which are covered within the EU's Copernicus services, specifically:

- The Climate Change Service (C3S);
- The Atmospheric Monitoring Service (CAMS); and
- The Marine Environmental Monitoring Service (CMEMS).

So the ECVs addressed are:

- Sea Surface Temperature (SST)
- Sea Surface Height (SSH)
- Sea Ice (SI)
- Soil Moisture (SM)
- Atmospheric Composition

The report begins with a review of the status for the ECVs addressed in WP4 (Section 2), followed by reviews of SST, SSH, SI, SM and Atmospheric Composition in Sections 3-7, respectively.

2. Temperature and Humidity

Background

Atmospheric temperature and humidity are fundamental state variables influencing the evolution of the atmosphere on timescales ranging from minutes to centuries. Accurate estimates of these variables are critical in providing the initial conditions for NWP models that form the basis of operational weather forecasts. On longer timescales, the accurate estimation of temperature and humidity has been used to determine trends associated with climate change, from solely observational datasets (McCarthy et al, 2009 , Sherwood et al, 2008) as well as from atmospheric reanalyses (Dessler *et al*, 2010, Simmons *et al*, 2014) .

Climate Data Records (CDRs) have typically taken the form of direct measurements of atmospheric temperature and humidity, for example from radiosonde measurements (Haimberger *et al*, 2014). More recently, increasing use has been made of estimates from atmospheric reanalyses. These atmospheric reanalyses make use of state-of-the-art NWP systems to provide consistent analyses of the global atmospheric state over many decades. They assimilate observations from the global observing system, often including higher quality reprocessed observational datasets than are available in near-real-time. These reanalyses attempt to combine the diverse range of observations available in an optimal way, given the uncertainty characteristics of the observations and the uncertainty characteristics of the forecast model, which is used to propagate the observational information forward in time from one analysis cycle to the next. Passive satellite observations in the microwave (MW) and infrared (IR) regions of the spectrum are of particular importance in analysing atmospheric temperature and humidity, although other observations (notably those from radiosondes and GNSS-RO) also play an important role. These radiance observations are assimilated directly, normally as top-of-atmosphere level 1 brightness temperatures. In recent years, much effort has been focussed on the development of Fundamental Climate Data Records (FCDRs) – Level 1 datasets of the highest quality achievable (Fennig *et al*, 2013).

The global observing system providing information on temperature and humidity has evolved considerably since the beginning of the modern meteorological satellite era (1979 onwards). Today, the constellation of satellites providing temperature and/or humidity information includes instruments operated by agencies in the US, Europe, Japan, China, India, Korea and Russia. Currently, global NWP centres will typically assimilate observations from 10-20 MW and IR instruments. In reanalysis, a similar set of observations will be assimilated. The prospects for the continuation of this comprehensive constellation are good, with firm plans in place by major agencies in the US, Europe and China to continue to populate and operate the constellation in its current form until around 2040. The continuation of these data records can present challenges though. As new technologies are developed, to reduce costs, size, mass and volume, whilst maintaining or improving radiometric performance, new bias characteristics are often evident in the data. This can present a challenge to meet the ever more stringent requirements of modern NWP systems and for the longer term development of FCDRs. As described below, the use of global NWP systems as part of the validation process for *new* satellites is now established. Analogously, the use of atmospheric reanalyses in assessing the quality of *reprocessed* satellite datasets is becoming more widespread.

Current approaches to validation

The technique of simultaneous nadir overpasses (SNO) has been widely used to assess inter-satellite biases in the development of FCDRs. SNO exploits the occasional spatio-temporal coincidence of sun synchronous polar orbiting satellites to quantify and correct inter-satellite biases. These coincidences generally occur in the polar regions, but for satellites in non-sun-synchronous orbits these coincidences take place at lower latitudes (the extended SNO technique – or SNO-x). As an example, Zou and Wang (2011) have used the technique to study inter-satellite biases in MSU and AMSU-A instruments. Using spatio-temporal colocation criteria of 65 km and 50 seconds, they found SNOs typically occur every 7-10 days. Zou and Wang invoke a number of parameters to model the diagnosed biases - including a global radiance offset, radiometer non-linearity and spectral shifts in the pass bands of channels. Estimated inter-satellite biases are significantly reduced using the technique.

Potential weaknesses of the technique are related to the limited geographical location of the SNO colocations, and the associated limited dynamic range of atmospheric and surface states sampled by SNO. In practice, however, this is not a serious issue for temperature sounding channels as the seasonal variation of atmospheric temperatures at polar latitudes samples most of the global range of temperatures for sounding channels. For humidity sounding channels, the sampling of solely drier atmospheric profiles at high latitudes is a more significant issue. The technique also makes an implicit assumption that the weighting functions for nominally identical channels are matched (with concomitant introduction of uncertainty if this assumption is violated). The technique has been effective in achieving improved inter-instrument homogeneity and has been used to identify long-term drifts in some satellite instruments (*e.g.* NOAA-16 AMSU-A).

Aircraft underflights have been used successfully in satellite validation campaigns. Aircraft provide mobile observation platforms to obtain measurements co-located with satellite observations. For the characterisation of satellite-radiance measurements, aircraft provide two means of validation:

- Direct comparisons of radiometric measurements made by airborne radiometers and satellite instruments. For window channels that are only weakly affected by atmospheric conditions, this offers a direct quantification of the differences between airborne and satellite observations. For example, during the JAIVEx campaign (Larar et al, 2010), it was shown that differences between IASI and an aircraft radiometer were around 0.1K in the 11 μm window region.

- Provision of co-located 'ground truth' observations in the form of dropsonde temperature and humidity profiles coupled with radiometric measurements of surface skin temperature. Above the aircraft flight altitude, atmospheric state can be obtained from NWP models. A radiative-transfer model is then used to map the measured atmospheric state to observation space and compared with the coincident satellite measurement.

In the former approach, this method can be developed further by using traceably calibrated aircraft radiometers to establish the absolute radiometric uncertainties in the aircraft radiometer and hence infer the absolute uncertainties in the satellite instrument. Tobin et al. (2013) have developed this concept and employed traceably calibrated airborne radiometers in the validation of observations from the Suomi-NPP CrIS radiometer. Absolute radiometric uncertainties are estimated to be 0.3K for the long wavelength channels of CrIS. This method is unique in enabling a determination of the absolute uncertainties in the satellite-radiance measurements, at least at the location of the colocation. A drawback of aircraft validation campaigns is that the geographical coverage of the colocations tends to be limited, and hence the scope to characterise complex, state dependent biases or orbital biases is limited.

Ground-based observations have formed part of satellite Cal/Val campaigns in recent years (Calbet et al, 2011). This aspect of Cal/Val is typically focussed on the validation of level 2 products although some of these campaigns have directly addressed the issues of bias and uncertainties in the level 1 radiance data from satellite instruments. The GRUAN network (Immler et al, 2010) aims to make high-quality measurements of atmospheric state at a number of sites globally. Establishing metrological traceability is a key aim of the network and this should ensure that absolute uncertainties can be determined for the observations made at GRUAN sites and, in turn, satellite observations validated through comparisons with the GRUAN measurements.

Several other, *non-NWP*, techniques are used in the validation of satellite sounding measurements. Satellite manoeuvres on-orbit, in which the spacecraft is rotated so that radiometers can directly view cold space, are used to assess biases due to instrument self-emission. For microwave imagers, views of radiometrically homogeneous and stable scenes, such as the radiometrically cold ocean surface, or rainforest scenes, have been used to assess the long-term stability of microwave instruments (Ruf, 2000).

Increasingly over the last decade though, NWP-based methods of characterising and validating new satellite temperature and humidity sounders have come to be seen as a very powerful tool. The value of using NWP models in characterising satellite observations stems from the high accuracy of current global NWP models. As indicated in the introductory section, this high accuracy results from a number of factors, including: the diverse range of high-quality observations used in the analysis; the efficiency of current data assimilation schemes is extracting information from the observations in a consistent way; and finally the high quality of current forecast models in propagating observation information between analysis cycles. For tropospheric temperature sounding channels, background errors (in observation space) are estimated to be in the range 50-100mK. For humidity sounding channels, the value is in the range 1-2K. As a consequence, computed first guess brightness temperatures are a good proxy for 'truth' in characterising new instruments. Two early examples of this approach, for SSMIS and FY-3A MWTS are given below.

The Special Sensor Microwave Imager/Sounder (SSMI/S, or SSMIS, Kunkee et al, 2008) followed the Special Sensor Microwave Imager (SSMI) series of instruments, which formed part of the US Defence Meteorological Satellite Program (DMSP) payload, successfully flown since 1987 (Colton and Poe, 1999). The first SSMIS instrument, on-board the DMSP F-16 satellite, was launched in October 2003. During the early phases of the Cal/Val campaign, SSMIS measured brightness temperatures were compared with simulations from NWP fields (both ECMWF and Met Office (Bell *et al*, 2008)). An analysis of first guess departure time-series revealed that two significant biases were evident in the SSMIS temperature sounding channels: gain anomalies caused by solar radiation impinging on the surface of the warm calibration load causing depressions of ~1K in the measured brightness temperatures, and; orbital biases caused by thermal emission from the main (emissive) reflector, which experienced temperature variations of 80K during an orbit, resulting in brightness temperature errors of ~1K. In a conventional microwave imager instrument without temperature sounding channels, these effects are much more difficult to detect. Nevertheless, it has been shown subsequently that imager missions have suffered similar biases due to emissive reflectors. Geer *et al* (2010), showed that TMI suffered similar biases due to reflector emission.

The first of China's latest series of polar orbiting meteorological satellites, FY3-A, was launched in May 2008 (Dong et al, 2009). The satellite carried several instruments of interest for NWP and reanalysis applications, including the Microwave Temperature Sounder (MWTS). MWTS is a cross track scanning four channel microwave sounder, with channels centred at 50.3, 53.596, 54.94 and 57.29 GHz. These are equivalent to AMSU-A channels 3, 5, 7 and 9. An NWP-based analysis showed that the variance of the first guess departures (observation minus model equivalents) could be substantially reduced by assuming significant frequency shifts for the MWTS channel centre frequencies. The shifts were in the range 30-55 MHz depending on channel. Radiometer non-linearities were also found to play a role in the biases evident for MWTS. Having corrected for these two effects, the MWTS data quality was significantly improved (Lu et al, 2011a) and proved beneficial when assimilated in the ECMWF forecasting system (Lu et al, 2011b). The approach was applied to data from MSU and AMSU-A microwave sounders, which showed strong evidence of passband shifts and drifts (Lu and Bell, 2013).

NWP-based analyses have also been carried out on the Suomi-NPP ATMS instrument (Bormann *et al*, 2013, Doherty *et al*, 2015). As part of WP4 detailed assessments of AMSR2, FY-3C MWHS-2/MWRI, Meteor M-N2 MTVZA-GY and GMI have been carried out and reports on these assessments have formed deliverables 4.2, 4.5 and 4.6.

Global analysis systems

Data assimilation systems are an integral component of operational NWP and have, consequently, benefitted from concerted research and development efforts over many decades at national and international meteorological centres. Temperature and humidity (or variables closely related to these) are explicitly analysed within these systems and provide the initial conditions for forecast model integrations. Currently, state-of-the-art global NWP models run at horizontal (grid-) resolutions of around 10km and employ data assimilation systems based on 4D-Var (Courtier *et al*, 1994, Rawlins *et al*, 2007). These systems typically assimilate observations from a diverse array of conventional and satellite observations, which, collectively, provide near-global coverage for most parts of the atmosphere in each assimilation cycle (of 6-12 hours typically). Ensembles of forecasts are commonly used to provide estimates of flow dependent uncertainties in the background fields used as prior constraints in variational assimilation schemes (Isaksen *et al*, 2010) .

The same, or very similar, NWP models are run at several centres in reanalysis mode, and in recent years new versions of these reanalyses are produced at 5-10 year intervals, in order to benefit from advances in NWP modelling, the availability of more powerful supercomputers (permitting reanalyses to be run at higher resolution using larger ensembles), as well as the availability of higher quality reprocessed datasets.

In WP4 of GAIA-CLIM, it was shown how NWP systems could be used to characterise and validate level 1 observations from new satellites. Model equivalents of measured satellite radiances, based on short-range forecasts (T+6 or T+12 hours), are able to characterise uncertainties in tropospheric temperature sounding channels at a level of 0.1 - 0.2K. For humidity sounding channels, the figure is around 1K, and for microwave channels, which are sensitive to the surface, the figure is 2-5K (limited by uncertainties in the radiative-transfer modelling of ocean surface emission).

Future evolution of global analysis systems

It can be expected that global analysis and forecasting systems will continue to advance steadily. A realistic expectation is that global models will run at around 5km (grid-) resolution by 2030, and that ensembles of forecasts and data assimilations will play an ever greater role in improving the estimation of uncertainties in model fields. The representation of moist processes in particular is expected to benefit significantly as a result of these developments. It is noteworthy that, as demonstrated in WP4, the misfit of short-range forecasts to humidity sensitive radiances (in clear sky conditions) in the Met Office global NWP model has improved significantly in the last decade: reducing from 2K in 2007, to 1K in 2017. This is partly a result of model improvements (including resolution upgrades and improvements to both data assimilation and forecast models) and partly as a result of the increased number of humidity observations constraining the analysis. Consequently it can be expected the value of using NWP-based approaches to the validation of new satellite sounding data for temperature and humidity data will continue to increase.

WP4 identified (and documented in the Gap Assessment and Impacts Document, GAID[1]) the need for improved modelling of radiative transfer at the (land and ocean) surface to improve the utility of NWP systems for the validation of surface sensitive satellite radiance measurements. This is a specific example of the general need for ongoing work to improve the observation operators linking model variables with observed quantities. The need for improved understanding of the spectroscopy in key regions of the microwave spectrum, such as at 183 GHz (Brogniez *et al*, 2016) and at 50-60 GHz, is another example captured in the GAIA-CLIM GAID.

In the context of the validation of historic data as part of the reprocessing of satellite datasets, the role of using atmospheric reanalyses as a tool for the evaluation of data quality (Kobayashi *et al*, 2017) is likely to increase.

Reference observation networks

Several of the observation types which are actively assimilated in global NWP systems, and in atmospheric reanalyses, *could* be considered to be of reference or *near*-reference quality. For example, GNSS-Radio Occultation observations (Healy, 2008), assimilated as bending angles, are derived from phase-delay (time) measurements, which have a short and direct traceability chain to the SI and consequently exhibit low bias characteristics. GNSS-RO measurements provide important information on temperature and humidity from the mid-troposphere to the mid-stratosphere. In addition, recent validation campaigns have shown the radiometric uncertainties of radiance measurements from the infrared interferometric radiometers IASI (MetOp-A and MetOp-B) and CrIS (Suomi NPP), which provide temperature and humidity information for NWP and reanalyses, have radiometric uncertainties of less than 0.3K. The variational bias corrections applied to these observations in NWP systems are typically less than 0.2K, implying the assimilation system is making adjustments to the uncorrected brightness temperatures that are consistent with the uncertainties

[1] http://www.gaia-clim.eu/page/gaid

in these observations. In summary – the high quality of many of the observation types assimilated in modern NWP systems (and reanalyses) have ensured the analysed fields are themselves of high quality.

Nevertheless, reference observations are normally considered to be *independent* datasets that can be used to assess the quality of other measurements or analyses. This has been an aim of the GRUAN network which currently comprises a global network of 22 sites (at 2016) worldwide with the aim of providing high-quality observations of variables, including atmospheric temperature and humidity. A key component of the network is high quality radiosonde observations. Dirksen et al (2014) have shown that the GRUAN (version 2) uncertainties in temperature range from 0.15K (night-time mid-troposphere) to 0.6K (daytime at 30km), whilst uncertainties for relative humidity are 6%. It is expected that the GRUAN network will continue in operation for the foreseeable future.

Within WP4, methods have been developed to use the GRUAN data to assess the uncertainties in NWP fields (in terms of temperature and humidity) as well as the uncertainties in brightness temperatures computed from the NWP fields.

Conclusions

The aim of this section of the report has been to describe the status of current practise in the validation of satellite observations of temperature and humidity. In particular, it has aimed to show how NWP systems have come to play a central role in the validation of new satellite sensors, and how the ongoing development of data assimilation systems, the observing network and reference quality observing networks will support the continued and improved use of NWP and reanalyses for the validation of new, and reprocessed, satellite datasets, respectively. The NWP-based validation approach will continue to be complemented by conventional approaches to validation (*i.e. e.g.* SNO and satellite-to-*ground-truth* match-ups).

The use of NWP-based approaches to the validation of temperature sounding radiances (for channels with minimal or no surface sensitivity) is well established. The application to humidity sounding data is already useful and improving rapidly, as demonstrated within WP4 of GAIA-CLIM. The application to microwave imager data, for which there is high surface sensitivity, although demonstrably useful, is hampered by remaining gaps in our understanding and representation of surface-radiative effects over ocean and land.

Further improvements in our understanding and representation of the fundamental spectroscopy and radiative transfer in key bands of both, the microwave (50-60 GHz and 183 GHz) and the infrared (in both longwave and shortwave CO_2 bands), will improve the utility of NWP for validation, as the radiometric uncertainties of state-of-the-art IR and MW instruments (currently around 0.3K) improve steadily. Both of these gaps (surface radiative transfer and spectroscopy) have been identified as part of the GAIA-CLIM gap analysis.

Finally, another purpose of this section has been to identify, and illustrate through the specific examples of temperature and humidity, the main *general* elements required for *any* global analysis system to be used effectively for the validation of satellite derived ECVs.

3. Sea Surface Temperature

Background

Sea Surface Temperature (SST) is an ECV extensively used in NWP and Earth sciences. The first SST measurements were derived from temperature measurements of sea water samples obtained using buckets (initially wooden, then canvas, and latterly rubber) from aboard sailing ships. SST records obtained in this way date back to the 1850s (Kennedy et al, 2011; Rayner et al, 2006). More recent in-situ measurements have been made from buoys, drifters, soundings, ship engine intake temperatures and in-situ radiometers on board research vessels (Donlon et al, 2002). Measurements from radiometers on-board satellites considerably increase the amount and variety of SST data available.

The ocean surface emits radiation at both infrared and microwave wavelengths that depends on SST. Satellite SST measurements are therefore available from both infrared (IR) and microwave (MW) sensors and are derived from the measured radiances using radiative transfer models. IR sensors measure the skin SST (with effective skin depths of ~10-20 µm) while MW sensors measure the sub-skin SST (with effective skin depths of ~1mm). Due to the complex and variable structure of the temperature in the upper ocean (cf. definitions by the The Group for High Resolution Sea Surface Temperature)[2], differences between the two types of measurement can be as large as 1K and need to be taken into account when comparing or combining IR and MW SSTs.

Thermal IR SST measurements are derived from radiometric observations at wavelengths of ~3.7 µm and/or 10 µm. The 3.7 µm channel is primarily used for night-time measurements to avoid contamination by reflection of solar irradiance. As both bands are sensitive to the radiative effects of clouds, only cloud free measurements can be used after atmospheric correction for scattering and absorption effects by aerosols and water vapour. When compared to MW sensors, IR SST measurements show better accuracy (when validated against in-situ measurements) and higher resolution (1 to 4 km for IR as compared to 25 km for MW) due to the lower signal strength of the Earth's Planck radiation curve in the microwave region. MW sensors are, however, largely unaffected by clouds and measurements at various frequencies permit the efficient removal of atmospheric and surface-roughness effects, thus providing a global picture of the SST.

SST measurements have been derived from a variety of IR sensors such as the Advanced Very High Resolution Radiometer (AVHRR), Advanced Along-Track Scanning Radiometer (AATSR) and Moderate Resolution Imaging Spectroradiometer (MODIS), for example. MW sensors include the Tropical Microwave Imager (TMI) and Advanced Microwave Scanning Radiometer (AMSR). The current EUMETSAT MetOp missions carry both AVHRR and IASI IR sensor that provides complementary measurements of SST and an accuracy better than 0.3K (O'Carrol et al, 2012). The second generation of geostationary MeteoSat use SEVIRI as IR sensor that can provides SST with an accuracy better than 0.5K (Merchant et al, 2009). The upcoming Copernicus Sentinel missions will use the SLSTR IR sensors which is a state-of-the-art version of the AATSR aiming for an accuracy better than 0.3K.

A number of missions are carried out on a global scale such as the NOAA series, GOES series, NASA's AQUA and TERRA, TRMM (NASA and JAXA), Suomi NPP, GCOM (JAXA), MTSAT (JMA), FY-3 (CMA), HY-1 and 2 (CAST). Future missions will include Copernicus sentinel (-3) missions, the new

[2] https://www.ghrsst.org/ghrsst-data-services/products/

generations of MeteoSat, the continuation of the NOAA series, OCEANSAT-3 (India), HY-3 (CAST) and GeoKOMPSAT (KMA).

Current approaches to Cal/Val

In-situ observations are used for the calibration and validation activities linked to satellite SST observations. They are used to initially calibrate the satellite SST algorithms (derive coefficients of the regression equation) and then to continuously validate the retrievals (monitor global statistics of “satellite minus in situ” SST differences). Satellite SSTs are collocated with in-situ data from buoys, drifters and on-board radiometers (Donlon et al, 2002) to determine both bias and root-mean square error. Three-way validation (or triple colocation) methods are using two different satellite instruments together with in-situ data to provide an error analysis (O’Carrol et al., 2008; Gentemann, 2014). When colocating data, the time and depth of the measurement as well as the atmospheric condition (especially wind speed) need to be considered to derive the correct SST value. Triple colocation gives root mean square errors (RMSE) of less than 0.3K, and around 0.4K, for IR and MW instruments respectively, and around 0.2K for in-situ buoys. Uncertainties depend on the instrument type and on both the atmospheric and oceanic conditions that affect the quality of both the retrieval and the uncertainties of the reference observations. Comparison of satellite SST observations with SST estimates from global-analysis systems is becoming more commonly used, for example through the SST Quality Monitoring (SQUAM) (Dash et al, 2010, 2012) developed in the context of the Monitoring & Evaluation of Thematic Information from Space (METIS) initiative coordinated by EUMETSAT and ESA.

Global analysis systems

Currently, most SST global analyses are observation-based (rather than model and observation based, as is currently the case with atmospheric data assimilation systems). They combine IR or/and MW SST estimates with in-situ observations. Most have some type of satellite bias correction using either in-situ data or one type of satellite data (or both) as a reference (Reynolds et al, 2010). The CMEMS OSTIA SST analysis (Donlon et al, 2012) currently uses an Optimal Interpolation (OI) scheme to combine SST measurements from IR and MW, as well as in-situ observations, to provide a 1/20 degree daily SST maps that are used operationally at both UK Met Office and ECMWF for NWP and climate-reanalysis applications. In OSTIA, both in-situ and measurements from the VIIRS sensor are used as a reference for bias correction. Validation activities showed that SST products have zero mean bias and uncertainty around 0.57K compared to in-situ measurements (Donlon et al, 2012). The ESA CCI SST analysis (Merchant et al, 2014) used the OSTIA framework to provide an SST analysis at 1/20 degree for climate studies based on IR sensors only (AVHRR and (A)ATSR). Validation against in-situ data showed a slight positive bias with uncertainties around 0.2-0.3K due to the use of a consistent dataset (IR sensors only). NOAA provides two high resolution (¼ degree) SST analyses products (Reynolds et al, 2007) based on an OI scheme (OIv2), one using AVHRR only and one using AVHRR and AMSRE. The NCEP RTG SST analysis (Thiebaux et al, 2003; Gemmill et al, 2007) also combines IR and MW sensors (AVHRR, GOES and AMSRE). It uses a 2D-Var scheme to provide daily global 1/12 degree SST analyses used operationally at NCEP. Validation against in-situ data gives uncertainties estimates around 0.6K, depending on the area of interest.

Most model-based ocean data assimilation systems use L4 SST products to constrain the first layer of the ocean. The ECMWF ORAS4/ORAP5 system (Balmaseda et al, 2013; Zuo et al, 2015) uses a nudging scheme that relaxes the ocean-surface temperature towards the OSTIA analysis in the recent years. The CMEMS operational analysis provided by Mercator Ocean (Lellouche et al, 2013) also uses OSTIA in the recent period. The CMCC C-GLORS (Storto et al, 2015) nudges SST towards the NOAA high resolution SST (OIv2, Reynolds et al, 2007). On the other hand, the FOAM system developed at the UK Met Office (Waters et al, 2015) assimilates the same SST data (along-track satellite and in-situ measurements) used to produce OSTIA in the NEMO framework using the NEMOVAR assimilation scheme. Validation of FOAM SSTs against in-situ observations and AATSR showed an uncertainty around 0.4K globally.

Evolution of global analysis systems

Future evolutions of the analysis systems for SST, both observation and model-based, will focus on resolution. High resolution SST analysis are already available such as OSTIA at 1/20 degree, NCEP RTG at 1/12 degree or NOAA OIv2 at ¼ degree. However the effective resolution of such products is made coarser during the analysis process (Reynolds et al, 2010). The MUR SST analysis (Chin et al, 2013) is a 0.01 degree product which is able to better capture fine-scale features using innovative variational techniques. Improving assimilation methods for SST analysis is an area of active research, the goal being a better representation of small-scale features such as SST gradients and eddies. Bias-correction methods are also evolving to better take into account measurement uncertainties in both satellite and ground-reference measurements (Merchant et al, 2014). This is crucial when combining measurements from different sources. The definition of SST being ambiguous, the GHRSST has defined a framework for the characterisation of the various SST measurements depending on depth and atmospheric conditions. These specifications are already adopted by most analyses and new products are expected to follow them in the future. Model-based ocean data assimilation is a relatively young field. More and more efforts are being focussed in developing high resolution ocean analysis systems as NWP centres, such as the UK Met Office and ECMWF, are moving towards an Earth system approach to NWP and reanalysis. The SST analysis provided by such systems is still let down by the representation of mesoscale features and western boundary current by ocean models and the lack of observational constraints, especially in the subsurface. Both ocean models and data assimilation methods are evolving towards a better representation of processes that matter for SST and NWP.

Regarding the use of passive IR and MW radiance data, in general, current and anticipated SST analysis systems assimilate high level (level 2 and above) SST products derived from the level 1 radiance (or brightness temperature) measurements. Potential gains in SST-analysis accuracy through the development of more optimal assimilation schemes are currently judged to be small and limited by the complexity of forward models (ocean foundation temperature to top-of-atmosphere radiances) and the large uncertainties in the variables required for accurate forward models at the (short) spatial scales (1 - 5km) of interest. Nevertheless, in the longer term, there may be incremental gains to be realised from the assimilation of level 1 products as global Earth system models move to km scale resolutions and represent many of the processes required for accurate forward modelling of level 1 radiances. There is likely to be a continued user requirement for SST estimates at km-scale resolution and accuracies below those currently attainable (~0.3K).

Reference observation networks

The requirement for reference quality observations of SST and ocean sub-surface temperature is recognised as a priority. In practice, temperature measurements from Argo floats are used in some communities as independent reference-quality observations (Merchant et al, 2014).

For remotely sensed radiometric measurements of SST, there are initiatives to improve the metrological traceability of ground-truth reference. For example, FRM4STS is an ESA funded project, to establish and maintain SI traceability of global Fiducial Reference Measurements (FRM) for satellite derived surface temperature product validation (Donlon et al, 2014; Meldrum, 2017).

Conclusions

Currently, colocation with in-situ observations is the preferred method for satellite SST Cal/Val activities. Triple colocation (MW, IR and in situ) is the most robust and accurate validation method, providing uncertainties for the in-situ observations as well.

The comparison of new satellite based SST estimates with estimates produced by global SST analysis systems is becoming more widespread as analysed SSTs improve in accuracy and spatial resolution. In comparison to the systems developed for atmospheric analysis, and current practise for satellite validation, many of the same elements are in place in the domain of SST: a comprehensive observing system comprising high quality in-situ and satellite observations; sophisticated global analysis systems running at high spatial resolution (5km) in both near-real-time and in reanalysis mode; and an evolving network of reference observations for both in-situ and remotely sensed measurements. Current uncertainties of the global analyses (0.3K in the best cases) are close to the capabilities of the highest specified satellite observing systems (0.1-0.3K).

It is therefore very likely that validation practises for SST will continue to make increasing use of global SST analysis systems for new satellite sensors.

4. Sea level

Background

The principle behind the sea-level measurement by satellites is relatively simple. Satellite radar altimeters transmit an electromagnetic signal to Earth, and receive the echo from the sea surface, thus providing a measurement of the satellite-to-ocean range. This measurement is affected by water vapour and/or ionisation. After correction, the final range is estimated. Knowing the satellite orbit, the height of the satellite with respect to a reference ellipsoid can be determined. The sea-surface height is the range at a given instant from the sea surface to the reference ellipsoid. The sea-surface height is estimated as the difference between the satellite height and the satellite-to-ocean range.

Different frequencies can be used for radar altimeters depending on the mission objectives and constraints. Ku band (13.6 GHz) is the best compromise between capabilities of the technology, available bandwidth, sensitivity to atmospheric perturbations, and perturbation by ionospheric electrons. C band (5.3 GHz) and S band (3.2 GHz) are more sensitive ionospheric perturbation, and less to the effects of atmospheric liquid water. Such bands allow the correction of the ionospheric delay in combination with the Ku band. Ka band (35 GHz) allows better observation of ice, rain, coastal zones, land masses and wave heights. It has a relatively large bandwidth that provides higher resolution, especially near the coast. It is also better reflected on ice. It is affected by tropospheric water and water vapour. Measurements are not available for precipitation higher than 1.5 mm/h. Dual-frequency altimeters correct for delay due to ionospheric electrons and can give estimates of precipitation rate.

The largest uncertainties in the altimeter measurement system are due to poor orbit determination, introducing uncertainties at wavelengths greater than 1000 km while the mesoscale signal is less affected. Multi-mission altimeter data sets have significantly reduced these uncertainties and improved the accuracy of the satellite sea level observations (to the centimetre level) (Le Traon, 2013; Verron et al, 2015; Ablain et al, 2017; Stammer, D. and Cazenave, 2017). The mean sea level ECV is the global average of the sea-surface height and its evolution over time is routinely monitored on the European level as part of the ESA CCI[3]. Currently, global and regional sea level trends uncertainties are around 0.6 and 1-2 mm/year, respectively. The objective is to reach 0.3 and 0.5 mm/year (Ablain et al, 2015).

There are currently 6 satellite altimeters in service. Jason-2 and Jason-3 (cooperation between CNES, EUMETSAT, NASA and NOAA) fly a circular non-sun-synchronous orbit with a 10-day repeat cycle but ground tracks with a 315-km-width at the equator. From July 2017, Jason-2 is operating on a lower orbit than Jason 3. Saral/Altika (CNES and ISRO) has a 35-day repeat cycle and is complementary to Jason-2 ground tracks. From July 2016, Saral is on a drifting orbit. Cryosat-2 (ESA) carries a SAR interferometric altimeter. It flies on non-sun-synchronous orbit with 92° inclination for observing the poles. Sentinel-3 (Copernicus/ESA) has similar ground tracks to Saral, but with a 27-day repetitive cycle. HY-2A (CAST) was on a 14-day repeat cycle orbit until March 2016 and then moved on a geodetic orbit with 168-day repeat cycle. Future missions will include the launch of CFOSAT (CNES and CNSA) in 2018, the next Sentinel-3 (ESA) and HY-2 (CAST) satellites and the JASON-CS (Copernicus, ESA, EUMETSAT, NOAA, CNES and NASA/JPL) series from 2020. The launch of the swath

[3] http://www.esa-sealevel-cci.org/

altimeter SWOT (NASA, CNES, CSA and UKSA) in 2021 should improve the coverage and resolution of the SSH measurement with respect to the currently-used profile altimeters (Fu and Ubelmann, 2014).

Current approaches to Cal/Val

Methods used for the calibration and validation of satellite-altimetry data can be separated in three categories:

- mono-mission analysis assessing the internal consistency of a single mission

Checks on the number of available measurements and their validity are performed. Crossover differences are used to estimate the uncertainty of the SSH measurement (Cheney et al, 1989). The SSH measurement is monitored along-track to control the consistency and the stability of the altimeter measurement.

- multi-mission analysis to detect drifts or biases

Cross comparison between satellites allows to calibrate new altimeters (Prandi et al, 2015) and detect inconsistencies in the altimetry record provided by the different missions. It also allows to provide consistent long-term record of the sea-level ECV (Dettmering and Bosch, 2013).

- comparisons with the tide gauge and buoy networks

Comparisons with tide gauges are made at dedicated calibration sites in order to determine absolute bias of the SSH measurement (Valladeau et al., 2012). Colocation with the global tide gauges network is also part of the Cal/Val procedure to detect drifts or jumps in the SSH record. Tide gauge sea levels are routinely monitored for low-frequency drifts drift by comparison to readings taken from tide staffs by a human observer. Tide gauges are able to determine global sea-level trends with an uncertainty of a few tenths of a millimetre per year (Douglas, 1991). Tide gauges are used to monitor the stability of satellite altimeters and detect potential drifts (Mitchum, 1998).

Global analysis systems

Objective analyses of satellite-altimeter data (Le Traon et al, 1998) use optimal interpolation techniques to provide global maps of SSH. The CMES SL TAC provides near-real-time SSH analyses at ¼ degree resolution using all the satellite missions available. The system acquires and synchronizes altimeter and auxiliary data. Missions are homogenized with the same models and corrections. The multi-mission cross-calibration process removes any residual errors and biases. Altimeter fields are interpolated at crossover locations and dates. Data are cross validated, filtered from residual noise and small scale signals and finally sub-sampled. An optimal interpolation is conducted merging all the flying satellites to produce SSH maps.

Model-based ocean analysis systems currently assimilate level 3 along-track sea-level observations (Balmaseda et al, 2013; Zuo et al, 2015; Waters et al, 2015; Storto et al, 2015, Lellouche et al, 2013). Such systems can provide SSH with an uncertainty of less than 10 cm (Waters et al, 2015; Zuo et al, 2015).

Reference Observation Networks

The main reference observation networks for sea level are based on tide gauge datasets. For example, 5 tide gauge networks (GLOSS/CLIVAR, SONEL, OPPE, BODC and IMEDEA) are used for validation of sea level from altimetry in the context of the CMEMS SL TAC (Prandi and Debout, 2016). Tide gauges being by definition located close to the coast, most of the ocean surface is uncovered by such measurements. The use of the Argo dataset and its near global coverage as a reference network has been investigated and showed interesting potential (Legeais et al, 2016). Maintaining the observing network as such is the minimum requirement to ensure the quality of the sea-level measurement from altimetry.

Conclusions

Currently, colocation with in-situ observations from tide gauges and multi-mission calibration are the preferred method for altimeter sea level Cal/Val activities.

Objective analyses of global sea level are already able to integrate new satellite measurement as part of the Cal/Val procedure (Dibarboure et al., 2011). The uncertainty of sea-level estimates from model-based analysis systems is progressively reaching the level of the current satellite altimeters (a few cm). As for SST, many of the elements for validation through global analysis systems are in place. The observing system gathers high quality in-situ and satellite observations and is constantly evolving. Global analysis systems are running at high spatial resolution in both near-real-time and in reanalysis modes allowing the ingestion of the new altimeter data.

Validation practises for sea level will most likely make increasing use of global analysis systems for new altimeters.

5. Sea Ice

Background

Sea-ice concentration (SIC) is the main sea ice satellite observation assimilated in global analysis systems. It is mainly measured by satellite passive microwave radiometry. Microwave sensors can detect sea ice throughout all seasons thus providing a consistent data record. Successive series of satellites have carried microwave radiometers since the 1970s. The Special Sensor Microwave Imager (SSM/I) on board the Defense Meteorological Satellite Programme (DMSP) series has been operating since 1987 at frequencies lower than 100GHz. The more recent Advanced Microwave Scanning Radiometer (AMSR) instrument and the Special Sensor Microwave Imager Sounder (SSMIS) also operate at <100 GHz. The SIC derived from passive microwave radiometers are affected by errors due to atmospheric absorption and emission, wind roughening over open water, anomalous ice and snow emissivity. While the errors in the open water limit are relatively easy to assess, this is much more difficult over sea-ice as a reference ice concentration must be determined from high-resolution imagery or field observations. SIC from passive microwave radiometers are relatively coarse resolution, which makes a precise determination of the ice edge challenging. Multiple algorithms which are able to derive the SIC from the measured sea-ice emissivity have been developed (Andersen et al, 2007). The intercomparison between the SIC retrieval from these various approaches provide an estimate of the SIC uncertainty (Ivanova et al, 2014). The current sensors providing SIC measurements include AMSR2 (GCOM-W1) and SSMIS (DMSP). Future missions will include a follow-on AMSR2, which will be on board the future GCOM-W2 satellite (2019 launch).

Current approaches to Cal/Val

Calibration and validation activities for satellite SIC are quite different from what is done for SST and sea level. They are not based on colocations between satellite tracks and localised observations. SIC from satellites is instead validated against high resolution manual ice charts (Andersen et al, 2007; Tonboe et al, 2016). The National Ice Centre (NIC) has been producing ice charts for both Southern and Northern Hemispheres for more than 40 years. Ice charts are produced manually from all available satellite imagery, in-situ observations from ships and aircraft and meteorological/oceanographic guidance data. The ice charts are composite charts of the ice conditions over a period, using any data up to 72 hours old, used for strategic and tactical planning for offshore and shipping activity. Maps are produced manually by analysts and SIC estimates rely on the subjective judgement of the analysts. The use of high-resolution data from SAR and/or IR sensors gives a more accurate description of the ice edge than passive microwave data. There is more attention to detail for the ice edge than for the central Arctic, as ships operate in ice-free areas. The differences between ice charts from different ice centres can be as large as 30%, especially at intermediate concentrations (Kreiner et al, 2017). The ice charts are primarily based on SAR data (Radarsat-2), together with IR-line scanners such as AVHRR and MODIS data.

The satellite SIC is compared with the ice charts in terms of total ice concentration given by the ice chart. Both products are projected onto a common grid and a cell-by-cell comparison is carried out. For each ice chart, the deviation between ice-chart concentration and satellite retrieval is calculated. The match between the satellite measurement and the ice chart concentration interval is computed.

From there, the bias and uncertainty of the satellite measurement are available. It is difficult, if not impossible, to provide accurate uncertainty estimates for the ice charts (Andersen et al, 2007), but the target uncertainty for satellite SIC is 10% in the Northern Hemisphere and 15% in the Southern Hemisphere with respect to the charts (source: OSI-SAF website[4]).

Another aspect of the Cal/Val activities is the intercomparison between sea-ice retrieval algorithms. There are tens of different algorithms to retrieve SIC from microwave emissivities. Ivanova et al (2014) give an extensive overview of the most commonly used algorithms. The authors show that some algorithms are more adapted to high-concentrations areas while others perform better for intermediate or low concentrations. They also suggest that the OSI SAF method, combining algorithms adapted to different concentration rates, is relevant for global SIC products. Comparisons between algorithms also allow to provide an estimate of the uncertainty of SIC data that can be used for model-based SIC data assimilation.

Global analysis systems

SIC analyses based on satellite observations only are produced by the National Snow and Ice Data Centre (NSIDC) and EUMETSAT's OSI-SAF. As mentioned above, data from passive microwave radiometers is used to produce gridded maps of SIC. These products have been used to produce SST and sea ice analyses (Reynolds et al, 2002; Rayner et al, 2003). The OSTIA SST and sea-ice analysis (Donlon et al, 2012; Roberts-Jones et al, 2012), for example, uses the 10-km resolution near-real-time OSI-SAF product. Gaps in the data are filled using spatial and temporal interpolation techniques or persistence, if no data is available for more than a certain amount of time. Hirahara et al (2016) used similar techniques to produce the sea-ice analysis used as lower boundary condition for the ECMWF ERA5 atmospheric reanalysis system.

Model-based sea ice analyses are more and more common with the advances in sea-ice modelling. Most SIC analyses are produced by coupled ocean-sea ice models that assimilate pre-processed SIC values (often already gridded) from OSI-SAF or NSIDC products (Zuo et al, 2015; Waters et al, 2015; Storto et al, 2015, Lellouche et al, 2013). Innovation statistics provide an estimate of the uncertainty with respect to the assimilated data. Both FOAM (Waters et al, 2015) and ORAP5 (Tietsche et al, 2017) systems, for example, provide a SIC analysis that fit the observations better than 5%.

However, like in the case of SST and sea-level, model-based SIC analyses are not commonly used in the Cal/Val activities for satellite sea level measurements. Sea-ice models are evolving quickly and are able to realistically represent more and more physical processes (Vancoppenolle et al, 2009; Hunke and Lipscomb, 2010). Sea-ice modelling and data assimilation can potentially provide high quality and high-resolution information to complement and validate satellite observations of SIC.

Reference Observation Networks

Independent reference observations for passive microwave SIC Cal/Val mainly come from ships, aircraft and SAR imagery. Visual observations of sea ice from ships can be very accurate and are

[4] The EUMETSAT Ocean and Sea Ice Satellite Application Facility (OSI-SAF) website address is http://www.osi-saf.org/

reported in ice diaries from dedicated cruises (Haas and Lieser, 2003; Lieser, 2005). Aircraft data are also very useful for sensor calibration (Comiso et al, 2003). SAR data from Radarsat provide high resolution SIC observations, but its use is restricted to the winter season and its quality is subject to the skills of the ice analyst (Kwok, 2002).

Conclusions

Currently, the preferred methods for satellite SIC Cal/Val activities are statistics of matches to ice charts and the inter-comparison of SIC retrieval algorithms.

Observation-based sea ice analyses are currently an extension of the satellite products using interpolation and persistence techniques to fill the gap left by missing data. The rapid evolution of sea-ice models will provide information on sea ice that is difficult to measure via the observing systems. Sea ice data assimilation is also developing fast and the accuracy of the SIC analyses is continuously improving. As for SST and sea level, many of the elements for validation through global analysis systems are in place. The observing system for sea ice is well maintained due to its operational applications and the economic impacts linked with sea-ice monitoring. Global analysis systems are running at high spatial resolution in both near-real-time and in reanalysis modes, allowing the ingestion of the SIC data from passive radiometers.

The difficulties associated with the observation of sea ice and the rapid progresses made by sea ice modelling and data assimilation suggest good prospects for the use of global analysis systems for the validation of SIC from satellites.

6. Soil moisture

Background

Soil moisture (SM) plays an important role in moisture and heat interactions between the land surface and the atmosphere, which makes it an important factor in NWP and climate models. SM fluxes are key components of the hydrological cycle, thereby influencing river discharge, floods, droughts and plant transpiration. The accurate representation of SM can benefit many applications, such as seasonal weather forecasts (e.g. Weisheimer *et al.* 2011), agriculture (e.g. Martínez-Fernández *et al.,* 2016) and operational flood forecasting (e.g. Wanders *et al*., 2014). In 2010, SM was endorsed as ECV by the GCOS Programme[5].

The water content of a shallow surface layer can be estimated from a low-frequency microwave signal in the 1-10 GHz range (Schmugge *et al*., 1983). The L-band (1.1– 1.7 GHz) is often considered the optimal wavelength to observe SM since higher frequencies are more susceptible to contamination from vegetation and atmospheric effects (Schmugge *et al*., 1983; Kerr *et al*., 2001). The three principal instruments used for space borne low frequency microwave measurements are synthetic aperture radars (SAR), radiometers and radar scatterometers. Three of the core missions encompassing these instrument measurements are (1) the European Space Agency (ESA) soil moisture and Ocean Salinity (SMOS) mission, (2) the joint European Organization for the Exploitation of Meteorological Satellites (EUMETSAT)/ESA MetOp mission and (3) the National Aeronautics and Space Administration (NASA) Soil Moisture Active Passive (SMAP) mission.

The SMOS mission was launched in 2009 and is the first mission dedicated to soil moisture retrievals (Kerr *et al*., 2007, 2010, Pinori *et al*., 2008). It features a passive interferometric radiometer that measures the thermal emission of the Earth (brightness temperature) at an L-band frequency of 1.42 GHz (21 cm wavelength), at full polarization and for incidence angles from 0 to 60°. The SMOS level 2 SM product is retrieved by inverting a radiative-transfer model, the so-called tau-omega model. Up to 5 cm depth of soil are sampled every 2-3 days, with an average horizontal resolution of about 40 km.

The EUMETSAT Advanced Scatterometer (ASCAT) active sensor on the METOP-A (2006-) and METOP-B (2012-) satellites is a real-aperture radar instrument measuring radar backscatter using a VW polarization in the C-band (5.255GHz) (Bartalis *et al*., 2007a). Schmugge *et al* (1983) estimated that C-band observations typically penetrate between 0.5 and 2.5 cm depth. ASCAT produces a triplet of backscatter coefficients from the different antenna beams on both sides of the METOP satellites. Backscatter is measured at various incidence angles, which enables the extraction of the yearly cycle of the backscatter-incidence angle relationship. This is a prerequisite to the removal of seasonal vegetation effects (Bartalis *et al*., 2007a, 2007b). The extraction of the level 2 SM product is based on the change detection approach (Wagner *et al*., 1999). The ASCAT level 2 SM product is the first near-real-time operational SM product and produces global soil moisture maps at both 50 km and 25 km resolutions and a sampling time of 1-3 days.

The SMAP mission was launched by NASA in 2015, with the aim of integrating an L-band SAR and a real-aperture L-band radiometer as a single observing system, thereby combining the strengths of active and passive remote sensing for mapping SM (Entekhabi *et al*., 2010a). The radiometer and radar share the same feed from a large 6 m diameter conically scanning antenna. SAR instruments actively observe L-band brightness temperature at high resolution (of the order 1-100 m). However,

[5] https://www.ncdc.noaa.gov/gosic/gcos-essential-climate-variable-ecv-data-access-matrix

they typically operate with narrow swaths, which limits the temporal frequency of their measurements. Furthermore, the backscatter is highly sensitive to speckle noise, surface roughness and vegetation. These inherent difficulties with SAR measurements make them unsuitable alone to map soil moisture for NWP and hydrological applications. One of the objectives of SMAP was to merge the radar and radiometer observations in order to achieve an SM product at an intermediate resolution of about 10 km, while approaching the accuracy and the temporal frequency of the radiometer. The disaggregation of brightness temperature is performed using a time series change analysis, which assumes a linear relationship between the brightness temperature and the spatially averaged radar backscatter measurement anomalies. The level 2 SM product is retrieved by inverting the tau-omega model using a similar technique to SM derived from SMOS brightness temperatures. The SAR instrument stopped working on 7 July 2015 due to a hardware failure, after collecting just two months of data. Nevertheless, the radiometer continues to function; since 2017 NASA has delivered (in beta release[6]) the SMAP high resolution product using Sentinel-1 data combined with passive SMAP data .

The SMOS and SMAP missions aim to provide soil moisture with an uncertainty of less than 0.04 m^3/m^3, which would allow acceptable estimates of SM surface fluxes for NWP and hydrological applications (Kerr *et al*., 2010). The SMOS level 2 SM product and level 2 ASCAT surface SM product have been validated using in-situ SM measurements by Albergel *et al*., (2012), amongst other studies. The two datasets demonstrated an average root mean square difference (RMSD) of about 0.08 m^3/m^3 and correlations coefficients of 0.53 for SMOS and 0.54 for ASCAT, averaged over more than 200 sites with contrasting biomes and climatic conditions over a one year period (2010). Al-Yaari *et al*., (2017) evaluated SMOS and SMAP level 3 products (retrieved using a multilinear regression approach) using in-situ observations from more than 400 stations around the world. They found quite similar overall levels of uncertainty between the two products but some differences in performance among the various networks. In both studies, the SM products performed best on average in semi-arid or arid regions, particularly over Australia (average correlations > 0.7). The ASCAT C-band backscatter measurements have to contend with substantially reduced sensitivity to SM in moderately vegetated areas (<3 kg/m^2), while L-band brightness temperature measurements are sensitive to SM up to about 5 kg/m^2, representing about 65% of the Earth's surface. Some of the vegetation signal in the ASCAT backscatter measurements is removed using the fixed seasonal correction applied during the change detection process and work is ongoing to allow for inter-annual variability (Vreugdenhil *et al*., 2016). The main drawback for the SMOS and SMAP products is radiofrequency interference (RFI), whereby anthropogenic L-band emissions interfere with the natural L-band emissions from the Earth. RFI degrades the accuracy of the SM retrievals and is prevalent over much of Asia and some parts of Europe and South America. The RFI factor could partly explain the similar performance of SMOS and SMAP by Albergel *et al*., (2012), despite L-band being considered a superior frequency to C-band for SM retrievals. It is worth mentioning that the L-band is a globally protected frequency and since the SMOS launch more than half the RFI sources over Europe have been localized and switched off and progress has been made to remove these sources in other parts of the world (Oliva *et al*., 2012).

The minimum requirement for future satellite missions is to continue the data time series started by previous missions, since data gaps are detrimental to all users. There is also a consensus among users for the need to increase the resolution and to maintain or decrease the uncertainty of the corresponding SM products. This is partly motivated by the need to keep pace with the increasing resolution of operational NWP models and the user requirements of hydrometeorological models for smaller scale processes, e.g., convective precipitation and runoff patterns. The ASCAT instrument is scheduled to last until at least the mid 2020s with the launch of Metop-C in 2018 (Wagner *et al*.,

[6] See https://nsidc.org/data/smap/smap-data.html.

2013). Future plans are already at an advanced stage concerning the instrument to succeed ASCAT, namely SCA on the second generation satellites of the EUMETSAT polar system (Lin *et al*., 2012), which will provide C-band scatterometer data for SM retrievals at a resolution of 25 km. There are also various ideas for follow-on missions to SMOS. For example, the proposed SMOS-NEXT mission would provide high resolution SM measurements of 4 km using a new concept for interferometric measurements (Soldo *et al*., 2013), but the viability of this technology is still being assessed. Recently, there has been interest in combining C-band and L-band data from scatterometers and radiometers with independent high resolution C-band SAR data from the ESA Sentinel-1 satellite to reach resolutions of the order 1 km. This follows the same reasoning for merging the SAR and radiosonde data in the SMAP mission. Encouraging preliminary results have been demonstrated assimilating SMAP and Sentinel-1 SAR in the NASA catchment land surface model (LSM) (Lievens *et al*., 2017) and by combining ASCAT-derived SM with Sentinel-1 SAR for high resolution soil moisture maps over Europe (Bauer-Marschallinger *et al*., 2017). The SMAP-Sentinel Level 2 SM product is described by Das *et al.* (2017).

Current approaches to Cal/Val

In-situ reference measurements

In-situ SM observations are commonly used as a reference for validating space borne SM measurements due to their accuracy and long-term legacy. Dorigo *et al*., (2011) summarizes several of the most common in-situ measurement techniques, including the gravimetric method (see e.g. Seneviratne *et al*., 2010), Neutron probes (e.g. Vachaud *et al*., 1977), Electromagnetic techniques (e.g. Robinson *et al*., 2008)) and Cosmic-ray neutrons (e.g. Zreda *et al*., 2008). The gravimetric method, which is the only established technique to provide direct measurements, derives the SM content from the difference in mass of a sample of soil before and after drying. This process is labor-intensive and destructive and is therefore impractical for frequent temporal sampling. Instead, the gravimetric method is used for long-term climate studies and to calibrate the other techniques, where the instruments provide indirect but automatic measurements with a high temporal resolution (typically hourly). These indirect methods are employed for most of the high quality SM networks around the world, including the OZNET in Australia (Smith *et al.*, (2012)), SMOSMANIA in France (Calvet *et al*., 2007, Albergel *et al*., 2008), REMEDHUS in Spain (Martınez-Fernandez and Ceballos, 2005), AMMA in Africa (Cappelaere *et al*., 2009, de Rosnay *et al*., 2009) and the SNOTEL/SCAN networks in the United States (Schaefer and Paetzold, 2000), amongst others. In total more than 500 stations provide in-situ SM data at depths typically ranging between 0.05 m and 1 m and starting as early as the 1990s. The International Soil Moisture Network (ISMN, Dorigo *et al*., 2011) provides a harmonized collection of the SM observations from most of the available networks. Incoming soil-moisture observations are automatically screened for abnormal outliers and normalized to volumetric units.

The estimated uncertainty of in-situ SM measurements, accounting for instrument errors and local representativeness errors from the calibration, is typically in the range 0.02-0.03 m^3/m^3. These values are generally less than the expected uncertainty of most space borne SM measurements, including the target uncertainties of the SMOS and SMAP missions (0.04 m^3/m^3). Progressively, the technology and calibration techniques are being refined to reduce the instrument and calibration errors, while also reducing the cost of the sensors (see e.g. Kizito *et al*., 2008). New networks are also being introduced, which is gradually improving the global spatial coverage. For example, the Rahm regional soil moisture network was introduced in 2017 in the Netherlands (Benninga *et al*., 2018). The network consists of 15 stations over an area of 240 km^2, measuring soil moisture using capacitance probes at several depths between 5 and 80 cm. The accuracy of the gravimetric calibration was enhanced by using soil-specific calibration functions, improving the estimated uncertainty from 0.03 m^3/m^3 to 0.02 m^3/m^3.

When comparing in-situ and space borne measurements, it is important to consider the vastly different spatial support between the two datasets (e.g. point-wise vs ~40 km). This is especially problematic given that SM can vary strongly over meters, for example due to variations in soil texture, topography or vegetation. It is therefore questionable whether the absolute difference between the two datasets has any value at all (Koster *et al*., 2009). For this reason, it is commonly assumed that the useful signal in the SM time series is a result of the temporal variability, rather than the absolute SM values (Entekhabi *et al*., 2010b). In line with this school of thought, it is necessary to rescale the SM datasets (reference and space borne) such that their climatologies are equivalent, either by using a linear rescaling (e.g. Albergel *et al*., 2012) or a cumulative distribution function (CDF) matching technique (Drusch *et al*., 2005; Reichle *et al*., 2007).

Triple colocation

A significant drawback with in-situ observations is their spatial coverage. Most networks consist of scattered sites in mid-latitudes, with huge gaps often between networks (hundreds of kilometers) and very little representation in the tropics and high latitudes. Therefore, it is not possible to provide complete uncertainty maps. For this reason, the comparison of satellite datasets with model simulations or with other satellite datasets for Cal/Val activities (e.g. De Jeu *et al*., 2008; Al-Yaari *et al*., 2014) will remain useful, even if there is ambiguity regarding the uncertainty of the reference dataset. The Triple Colocation (TC) method is designed to overcome this problem by estimating the unknown uncertainty variances of three colocated mutually-independent datasets, without treating any one dataset as the reference or "truth". Importantly, TC assumes that the datasets' uncertainties are uncorrelated with each other. It has been employed in many different applications, including evapotranspiration (Rosema, 1993), before being adopted in the SM context by Scipal *et al*., (2008). Since then, numerous SM studies have used this validation tool (e.g. Miralles *et al*., 2010; Draper *et al*., 2013). TC is often applied to SM anomalies rather than absolute time series, as they fit better with the underlying assumptions of the method (Miralles *et al*., 2010). So far, the TC method has been applied primarily to surface SM. Most space borne instruments measure only the first few centimeters of SM, which limits the available datasets for validating the root-zone to in-situ observations and model simulations. Furthermore, the root-zone SM is characterized by very slow temporal dynamics with typically variations at the annual scale for the first meter of soil. This contradicts a basic assumption of the TC theory, which assumes products have randomly distributed uncertainties. Nevertheless, Pellarin *et al*. (2013) showed interesting results on preliminary TC usage for root-zone SM validation. Further research would be required to make the method suitable for root-zone and slow varying products validation.

Global analysis systems

The ingredients for global SM analysis systems generally consist of LSMs and a combination of remotely sensed near-surface SM observations and/or screen-level observations of temperature and humidity. Due to their sparse spatial coverage, in-situ SM observations are limited to validation applications. Data Assimilation (DA) is used to interpolate and extrapolate the observations and to merge the information content with the LSM. Additionally, DA takes advantage of the dynamics of the model to spread the information content from the observations in space and time, including a vertical transfer of information from the surface to the root-zone (Reichle *et al*., 2002; Sabater *et al*., 2007). The resulting SM analysis has a complete spatial coverage at the model resolution, but in theory with reduced uncertainty relative to the model or observations alone.

Before the advent of near-real-time, global-scale space borne SM measurements, screen-level measurements (2 m temperature and relative humidity) from the SYNOP network were assimilated indirectly into operational soil moisture analysis systems. Mahfouf (1991) demonstrated that short-term forecast uncertainties in screen-level variables can be used to infer SM corrections using a 1D-optimal interpolation (OI) DA method. For instance, the OI method would interpret an underestimation in screen-level temperature (positive increments) as an overestimation in SM (negative increments) and vice-versa. In 1999, the European Centre for Medium Range Weather Forecasts (ECMWF) introduced their operational OI system (Douville *et al*, 2000; Mahfouf *et al*, 2000), which was active until 2010. The OI method was widely accepted at most NWP centres and is still operational at some NWP centres, including Meteo France (Giard and Bazile, 2000). Its popularity stemmed from the fact that it improved the accuracy of NWP forecasts in the lower boundary layer. In contrast, there is some evidence at ECMWF that it degraded the accuracy of the soil moisture analyses due to unrealistic SM increments (Drusch and Viterbo, 2007). Also, it is not flexible enough to assimilate new observation types, including space-borne measurements. Consequently, most operational centres have either introduced or are moving towards flow-dependent DA methods, which have dynamic background error covariances[7] and are flexible enough to assimilate both screen-level data and space borne SM measurements. The flow-dependent methods used in global land surface analysis systems are mainly based on the Extended Kalman Filter (EKF, Jazwinski, 1970) or the Ensemble Kalman Filter (EnKF, Evensen, 1994).

At ECMWF, the Simplified Extended Kalman filter (SEKF) was introduced in operations in 2010 to assimilate screen-level variables (de Rosnay *et al*., 2013) and has been assimilating ASCAT-derived SM since 2015 (ECMWF, 2015). The current resolution of the ECMWF global model is 9 km. The ASCAT data are mapped to the nearest model grid point, and CDF-matching is used to rescale the observation into volumetric SM (the model is not rescaled). The UK Met Office employs an SEKF to assimilate the same observation types using a similar approach (Candy *et al*., 2012). The SEKF method uses a fixed background error covariance at the start of each assimilation window, but generates implicit flow-dependence through the assimilation window via additional model integrations in the calculation of the observation operator Jacobians. At ECMWF, de Rosnay *et al*. (2013) demonstrated that the SEKF produces marginally better surface SM analysis scores compared with the OI method when validating against in-situ observations from the SMOSMANIA network in France, with average correlations of 0.84 for the SEKF and 0.80 for OI over January to November 2009. Other advantages of the SEKF over OI were highlighted, including smaller and more realistic analysis increments in the root-zone. In the aforementioned study by Albergel *et al*. (2012), the SMOS and ASCAT-derived SM products were also compared with an offline version of the SM analysis at ECMWF. The SEKF was configured to assimilate both ASCAT-derived SM and screen-level variables into the H-TESSEL LSM at 25 km resolution. The surface SM analysis demonstrated a superior accuracy relative to the space-borne measurements (validated against in-situ observations), with a CC (RMSD) of 0.70 (0.07 m^3/m^3) relative to 0.53 (0.08 m^3/m^3) for ASCAT and 0.54 (0.08 m^3/m^3) for SMOS. At NASA, the assimilation of SMAP in the catchment land surface model using an EnKF

[7] The GAIA-CLIM guidance note 'Guide to Uncertainty in Measurement & its Nomenclature' (http://www.gaia-clim.eu/sites/www.gaia-clim.eu/files/document/d2_6_final.pdf) cautions that 'error' and 'uncertainty' are not synonyms. Accordingly, in this report we have used 'uncertainty' to describe a probability distribution from which the (unknown) error on the measured value is drawn. The term 'error covariance' has a specific meaning in data assimilation, usually denoting the (co-)variance of expected error represented by a (routinely Gaussian) probability density function.

was evaluated for the period April 2015 to November 2016 (Reichle *et al*., 2017). Core validation sites were selected at 38 locations based on a number of criteria, including dense sensor networks and well documented intensive field campaigns. The SM analyses (SMAP level 4) in the root-zone compared very well with the in-situ observations at these sites, with an unbiased RMSD of 0.038 m^3/m^3, thereby meeting the target uncertainty of the SMAP mission (0.04 m^3/m^3).

High quality soil moisture reanalyses have been developed for climate studies and for validation purposes. Examples include the ERA-land reanalysis developed at ECMWF (Balsamo *et al*., 2015). The ERA-land is an offline land surface model simulation forced by ERA-interim atmospheric conditions (Dee *et al*., 2011) from which the precipitation forcing was corrected by high quality monthly averaged precipitation provided by the Global Precipitation Climatology Project (GPCP). It has since been used as a benchmark in the evaluation of new and existing SM products. For instance, Albergel *et al*. (2013) compared ERA-land with a microwave based multi-satellite SM dataset (SM-MW) over the time period 1980-2010. The SM-MW represents a blended contribution of passive products such as SMMR and AMSR-E (1980-2010) and more recent active products from the ERS and ASCAT scatterometers (1992-2010). It was found that the ERA-land and SM-MW became more consistent with each other over time, especially after the incorporation of the active satellite data (correlations increasing from 0.52 ± 0.1 to 0.66 ± 0.04). This evidence reinforces the need to expand the satellite network and to combine different space borne SM products in order to obtain more accurate SM maps. Indeed, a state-of-the-art blended space borne product has been developed by ESA's CCI, consisting of a combination of reprocessed passive and active microwave SM retrievals going back to 1979 (Liu *et al*., 2012; Gruber *et al*., 2017; Dorigo *et al*., 2017).

Evolution of global analysis systems

Operational SM analysis systems are being adapted to assimilate L-band space-borne measurements operationally. Muñoz-Sabater (2015) demonstrated the assimilation of SMOS level 1c brightness temperature using the SEKF in an offline version of the ECMWF land data assimilation system (LDAS) over a 15-day period. The results were encouraging, although it was acknowledged that longer validation studies would be required to properly evaluate the product. The SMOS level 2 SM product is retrieved by finding the soil moisture and vegetation characteristics that minimize a cost function of the difference between modelled direct and observed angular brightness temperature. A major drawback of this process is the computing time taken to minimize this cost function, which means the SM product cannot be ready in near-real-time for operations. An alternative SMOS SM product has been derived using a fast inversion with a neural network (SMOS NN) trained on SMOS level 2 SM (Rodríguez-Fernández *et al*., 2017). SMOS NN is available within 3.5 hours of sensing, which is well within operational time constraints. Rodríguez-Fernández *et al*., (2017) found that SMOS NN data agreed with SMOS level 2 data to within an uncertainty (standard deviation of the difference) of 0.05 $m^3\ m^{-3}$ over most of the globe. There are now plans to assimilate SMOS NN (trained on ECMWF LSM) operationally, together with ASCAT level 2. At NASA, a similar technique has been employed by Kolassa *et al*., (2017) to assimilate a version of the SMAP product derived from a neural network trained with the NASA land surface catchment model. An EnKF was used to assimilate the data into the LSM. The comparison with in-situ data showed a marginal improvement in SM scores when compared with the assimilation of SMAP level 2.

NWP systems are generally moving towards greater coupling between the different components, including the land, atmosphere and oceans. In most NWP centres, the land surface DA is weakly coupled to the atmospheric DA. This implies that the analysis corrections in each component influence the other components through the short forecast between assimilation cycles. One way to improve the flexibility and coupling between the systems is through ensemble DA. Currently, most leading NWP centres are not using ensemble DA methods to analyze SM. Ensemble DA is practical and effective in global analysis systems with very large model state dimensions, such as atmospheric NWP models (of the order 10^8 degrees of freedom), as it avoids the need to store or invert very large matrices for the Kalman gain computation. But land surface DA systems are not affected by the so called "curse of dimensionality", as LSMs are typically pointwise and consist of between 3 and 10 vertical layers, equating to model dimensions of the order 10 or less. An SEKF system is simpler to implement than an ensemble DA system as less calibration is required, and many offline studies have indicated similar levels of performance between the EKF and the EnKF methods (e.g. Reichle *et al*., 2002, Fairbairn *et al*., 2015). However, new opportunities are emerging for ensemble DA in coupled systems. Carrera *et al.* (2016) developed an operational EnKF for the Environment Canada land-surface model using an ensemble of precipitation forecasts from their NWP system to represent the uncertainty in the precipitation forcing. This was shown to improve the representation of uncertainty in the SM prior state pdf. At ECMWF, there are plans to replace the observation operator Jacobians of the SEKF with an ensemble of data assimilations (EDA) from the atmospheric analysis. This should enhance the flow-dependence of the DA system, while strengthening the land-atmosphere coupling.

The resolution of NWP systems will continue to increase in accordance with computing constraints. For example, the resolution of the operational NWP model at ECMWF has increased from 40 km in 2006 to 9 km in 2017. Future resolutions of the order 5 km (NWP and ensemble systems) and 1 km (offline runs of the land surface model) should enable the better representation of small- scale processes such as convective precipitation and runoff patterns, which would particularly benefit agriculture and flood forecasting. Work is also underway to build the successor to ERA-land, namely the ERA5 reanalysis. This will have a 31 km resolution as opposed to the 79 km resolution for ERA-land. It has already been released for a recent period (2010-present) and will be extended back to 1979. This will take advantage of the current advanced land surface DA scheme at ECMWF to assimilate processed space borne scatterometer measurements since 1992. The ERA5 SM analysis will provide an enhanced benchmark with which to compare new and existing SM products. A similar type of reanalysis has been setup by NASA (MERRA-land) and provides SM maps from 1980 onwards (Reichle *et al*., 2011).

Conclusions

Over the last decade, the availability of remotely sensed SM measurements has massively increased with the launch of the MetOp, SMOS and SMAP satellite missions, with resolutions of about 25-50 km. In particular, L-band measurements from the SMOS and SMAP missions are providing a wealth of new data that can be used to enhance SM maps and global analysis systems. It is important to validate this data to assess its accuracy and to highlight potential flaws that need to be addressed. Since the 1990s, in-situ SM observations have provided the most accurate and consistent reference for validation studies. In-situ measurements typically have uncertainty in the range 0.02-0.03 m^3/m^3, which is superior to the target uncertainty of the SMOS and SMAP satellite missions (0.04 m^3/m^3). The harmonization and standardization of the input data from the various networks of in-situ observations has been accomplished through the International Soil Moisture Network (ISMN) data hosting facility. Studies have gained insight into the uncertainty of SMOS, SMAP and ASCAT products by validating them against in-situ data in various parts of the world, with contrasting biomes and climate conditions. For example, it has become apparent that the SM derived from C-band ASCAT data is less accurate in highly vegetated regions. Regarding SMOS and SMAP, one of the main flaws is RFI, which originates from illegal anthropogenic L-band emissions. This has prevented useful SM measurements in much of Asia and parts of Europe. A concerted effort has since been made to locate and switch off the RFI sources. Future satellite missions will focus on achieving higher resolutions and continuing the data time series. New techniques combining SAR data with radiometer or scatterometer data could potentially achieve resolutions below 10 km, although further validation is needed.

In-situ observations are insufficient alone to validate SM products. Although accurate, they are sparsely located and missing completely from certain parts of the world, including the tropics and high latitudes. Complementary studies are used to check the consistency between different model simulations and datasets. In the absence of a clearly superior dataset that can be considered as a reference, the TC method has become a popular and effective technique to approximate the uncertainty in three different datasets, assuming they are uncorrelated with each other.

High-quality reanalyses with complete coverage can also be used as a benchmark to assess the global uncertainty of new and existing SM products. For example, the ERA-land reanalysis at ECMWF has been used as a benchmark to assess the uncertainty of blended satellite products between 1980 and 2010. Amongst other evidence, this has confirmed that combining satellite data from active and passive sensors enhances the resulting uncertainty of SM maps relative to individual sensors, which has led to the release of the ESA-CCI blended product (mapping from 1980 onwards). New SM reanalyses have been developed based on advanced DA systems, including ERA5 at ECMWF and MERRA-land at NASA.

Global soil moisture analysis systems are evolving to assimilate new observation types. The fast retrieval of SM from L-band passive measurements using neural networks will enable the near-real-time release of the SM products for operations. For example, ECMWF are planning to assimilate SMOS SM data derived from a neural network, in combination with the currently assimilated ASCAT-derived SM. Ensemble DA systems are being advocated to increase the flow-dependence of estimated uncertainties in the prior state and to strengthen the land-atmosphere coupling. This should improve the uncertainty of the resulting SM analysis, together with increasing model resolutions.

7. Atmospheric Composition

Background

Some of today's most important environmental concerns relate to the composition of the atmosphere. The increasing concentration of greenhouse gases and the cooling effect of aerosol are prominent drivers of a changing climate, but the extent of their impact is still uncertain.

At the Earth's surface, aerosols, ozone and other reactive gases such as nitrogen dioxide determine air quality, affecting human health and life expectancy, the health of ecosystems and the fabric of the built environment. Ozone distributions in the stratosphere influence the amount of ultraviolet radiation reaching the surface. Dust, sand, smoke and volcanic aerosols affect the safe operation of transport systems and the availability of power from solar generation, the formation of clouds and rainfall, and the remote sensing by satellite of land, ocean and atmosphere.

To address these environmental concerns there is a growing requirement for observational data and processed information. Within Europe, the Copernicus Atmosphere Monitoring Service (CAMS) has been developed to meet these needs.

CAMS delivers a range of operational services, including several which draw upon the operational analysis of air quality and atmospheric composition:

- Daily production of near-real-time analyses and forecasts of global atmospheric composition
- Daily production of near-real-time European air quality analyses and forecasts with a multi-model ensemble system
- Reanalyses providing consistent multi-annual global datasets of atmospheric composition and European air quality with a frozen model/assimilation system
- Greenhouse gas surface flux inversions for CO_2 , CH_4 and N_2O, allowing the monitoring of the evolution in time of these fluxes
- Climate forcings from aerosols and long-lived (CO_2 , CH_4) and shorter-lived (stratospheric and tropospheric ozone) agents
- Anthropogenic emissions for the global and European domains and global emissions from wildfires and biomass burning

Regarding the measurement of atmospheric composition SO_2, for example, has been measured from space since the 1982 eruption of El Chichón (Krueger, 1983; Krueger et al., 2008) using UV-VIS sensors. Those measurements were made by the Total Ozone Mapping Spectrometer (TOMS), which had a limited SO_2 detection sensitivity, since the discrete measurement wavelengths were designed for total ozone retrieval (Gurevich and Krueger, 1997). Since then, next-generation space-borne spectrometers such as GOME (Global Ozone Monitoring Experiment), GOME-2, SCIAMACHY (SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY) and OMI (Ozone Monitoring Instrument) have shown greatly improved SO_2 detection sensitivity.

Measurements of atmospheric methane from space have been made for the last two decades using both solar back-scattered radiation (*e.g.* SCIAMACHY and GOSAT) as well as thermal emission (IMG, AIRS, TES, IASI and CrIS). Missions based on active (lidar) techniques, as well as missions based on Geostationary satellites are currently under consideration (Jacob, 2016). In Europe, the planned Low

Earth Orbit satellite Senitinel-5, and the geostationary mission Sentinel-4, will target a range of key compounds including methane using solar backscatter in spectral ranges covering the UV from 270nm to the short wave infrared at 2.385 µm. The Tropospheric Monitoring Instrument (TROPOMI), also measures solar backscattered radiation and is carried on the Copernicus Sentinel-5 Precursor (-5P) mission, launched in October 2017. In addition to methane, TROPOMI also measures column ozone, nitrogen dioxide, methane, carbon monoxide, sulphur dioxide and formaldehyde (De Smedt, 2015).

The accurate measurement of column CO_2 has long been recognised as a key challenge in deriving anthropogenic and biogenic surface fluxes of CO_2 (Kort, 2012). Dedicated CO_2 monitoring missions have been launched in the last decade, using differential reflectance techniques in the shortwave infrared to derive accurate CO_2 columns. These missions include GOSAT (Kuze, 2009 and 2016, Hammerling, 2012), TANSAT (Liu, 2013) and OCO-2 (Eldering, 2017).

The growing importance of monitoring the impact of international protocols covering greenhouse gas emissions over the next century means that it is likely there will be strong and ongoing multi-agency commitment to operate satellite systems measuring greenhouse gases, and atmospheric composition more generally, for the foreseeable future.

Current Approaches to Cal/Val

Calibration and validation activities have traditionally made use of colocations with high quality measurements, some of reference quality, at a limited number of ground-based sites. SO_2 measurements from space, for example, have been validated using colocations with Brewer spectrophotometers. Typical levels of agreement are ± 2 DU (Ialongo, 2015)

Validation of the complete suite of CAMS products is carried out on an ongoing operational basis and validation reports are produced quarterly as part of the service (Eskes, 2017), drawing upon a wide range of reference datasets.[8]

Global analysis systems

Within CAMS a global analysis and forecasting system is run at a resolution of 40 km (T511) with 60 levels in the vertical. The system is integrated within the Integrated Forecasting System (IFS), a system originally developed as a Numerical Weather Prediction (NWP) model at ECMWF. The system generates forecast output at 3-hourly intervals, and incorporates treatment of a range of greenhouse gases, reactive gases and aerosols. A range of satellite observations are assimilated in the CAMS models: O_3 analyses are determined by observations from MLS, OMI, SBUV-2, OMPS and GOME-2; CO is constrained by observations from IASI and MOPPITT (Emmons, 2002, and Yurganov, 2008); SO_2 from GOME-2; and aerosol optical depth (AOD) observations from PMAP and MODIS are assimilated.

The greenhouse gas modules account for biogenic (Bousetta, 2013) and anthropogenic fluxes, ocean fluxes and fire related fluxes. CH_4 fluxes are prescribed from inventories and climatological datasets.

[8] See https://atmosphere.copernicus.eu/quarterly_validation_reports.

Reactive gases are treated by an extended version of the CB05 chemical scheme (Yarwood, 2005). The assimilation of aerosol optical depth data is described in Benedetti (2008).

Evolution of global analysis systems

Within Europe, as part of the operational CAMS service, the ongoing development of composition analysis and forecasting capability is anticipated for the foreseeable future. In the short term future there are plans to extend the assimilation of observations to include those from: the Sentinel-5P TROPOMI mission (O_3, NO_2, SO_2, CH_4 and CO); IASI (O_3); VIIRS (AOD and fire radiative power); and SEVIRI (AOD). In the longer term it is likely that the system will see continuous improvements in accuracy through: model developments in both analysis and forecasting aspects; higher resolution, enabled through advances in computing power; as well as the continued development and expansion of the observing system through significant contributions from all major satellite agencies.

It is likely that the system, or a similar system, will be further developed to support the operational estimation of regional anthropogenic CO_2 emission fluxes in support of international protocols aimed at monitoring and curbing greenhouse gas emissions. A key component of such systems will be the assimilation of observations from satellite sensors such as TANSAT and OCO-2 and future generations of similar instruments.

Reference Observation Networks

Several ground-based networks have been established in recent years to provide reference quality measurements, primarily aimed at the validation of space-based remote sensing measurements of atmospheric composition. The Network for the Detection of Atmospheric and Climate Change (NDACC, De Mazière, 2017), for example, comprises eighty sites equipped with a suite of complementary in-situ and remote sensing instruments including ozone sondes, Brewer, Dobson and UV-VIS spectrophotometers, microwave radiometers, Fourier Transform Infrared Spectrometers and Lidars. The quality of the observations is ensured through a refined set of measurement protocols and procedures, including regular inter-comparison campaigns. Due to its maturity, NDACC is among the networks that are recognized by the European Copernicus initiative as key networks for providing data for validation of the Copernicus Atmosphere Monitoring Service.

The Total Column Carbon Observing Network (TCCON) network fulfils a similar role for the monitoring of total column CO_2 and comprises network of high resolution Fourier Transform Infrared Spectrometers operating in the short wave infrared. (http://www.tccon.caltech.edu/index.html)

In the context of aerosol measurements, an analogous role is played by the AERONET (AErosol RObotic NETwork) project – a federation of ground-based remote sensing aerosol networks established by NASA and PHOTONS (PHOtométrie pour le Traitement Opérationnel de Normalisation Satellitaire) and augmented by other national networks. The project has provided a long-term, continuous and readily accessible public domain database of aerosol optical, microphysical and radiative properties for aerosol research and characterization, and for the validation of satellite observations for the last 25 years. In common with NDACC, the network imposes a standardization of instruments, calibration procedures, processing and distribution.

Validation of the complete suite of CAMS products is carried out on an ongoing operational basis and validation reports are produced quarterly as part of the service (Eskes, 2017), drawing upon a wide range of reference datasets.[9]

Conclusions

As outlined above, all of the key elements required to enable global analyses to be used as a component of the future validation of satellite observations of atmospheric composition are already in place, specifically:

- mature networks of reference quality ground-based observations (NDACC, TCCON, AERONET);
- sophisticated global analysis systems (e.g. in Europe, the IFS);
- assured evolution of those analysis systems;
- and a steadily growing constellation of satellite instruments targeting composition measurements.

Work is already ongoing to assess the value of global analyses in the validation of satellite data, and this approach is likely to become more widely used as analysis systems improve.

[9] https://atmosphere.copernicus.eu/quarterly_validation_reports

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