

REPORT

Data Set Quality Assessments:

Needs, Benefits, Best Practices and Governance

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Jörg Schulz, EUMETSAT, Chair GEWEX Data and Assessment Panel Peter Gleckler, Lawrence Livermore National Laboratory and many WCRP contributors hereby deeply acknowledged

1. Introduction

This document addresses the need for systematic assessments of the quality of data sets used in various applications such as climate services as well as climate science, including their use in the evaluation of climate model performance. The purpose of this document is to initiate a discussion within WCRP as to how the core projects, working groups and WCRP Grand Challenges can initiate data set quality assessments in a more coherent way, ensuring that the outcomes of assessments are beneficial for their own activities and also for activities across WCRP.

The scope of this discussion paper is limited to a description of the general benefits, high level practices, and potential governance structures for data set quality assessments. Detailed best practices are not included as part of this document because they depend too much on the actual physical system and data sets that are being assessed. The document is entirely based on experience garnered from conducting data set quality assessments for more than two decades within several WCRP core projects.

The document provides a brief description of the background from which the need arises and a short, but not exhaustive history of data set assessments as they were performed in GEWEX, CLIVAR, SPARC and elsewhere. It then lists the currently known types of assessments and the benefits that were drawn from them. The last set of sections proposes high-level best practices and addresses funding needs and governance issues.

2. Background

Climate variability and long-term changes in climate pose significant challenges to societies. The availability and communication of climate information through climate services significantly supports prevention of economic setbacks and humanitarian disasters. In addition, climate services play a critical role in national development planning, managing development opportunities and risks, and in mitigating and/or adapting to changes in climate. To provide authoritative information to all of these areas it is necessary to develop the best possible understanding of the quality of climate observations and derived products. Formalized, impartial, data set quality assessments are one way to analyse the fitness-for-purpose of climate data sets and can play a crucial role in the acceptance process of climate data products for climate services.

Comprehensive assessments of the physical science basis of climate change conducted by the Intergovernmental Panel on Climate Change (IPCC) refers to detailed scientific assessments of observations of various aspects of the climate system, with dedicated consideration of specific areas such sea level change, biogeochemical cycles, clouds and aerosols, and regional climate phenomena. Measurements are used to assess the status of the climate and to evaluate climate model simulations for the past to build confidence in model projections for the future. The use of measurements throughout the IPCC report is based on peer-reviewed publications about the individual climate data records (CDRs) and sometimes on comparison of CDRs. The IPCC Working

Group I report (IPCC, 2013), in particular chapter 2, provides comparison of a limited number of data records whereby the selection of particular CDRs depends on the expert knowledge of the authors. Only in one case does the IPCC refer to a publication related to a WCRP GEWEX assessment which is the cloud data set assessment (Stubenrauch et al., 2013). IPCC assessments reveal important geographical and temporal gaps in observations, understanding of system processes, and confidence in observations and projections themselves. However, IPCC assessments could, and should, make much more extensive use of community-wide assessments of the quality of existing CDRs, which could be provided under the leadership of WCRP, in particular the WCRP Data Advisory Council (WDAC).

A specific activity to facilitate the comparison of satellite observations with climate model data is the Observations for Model Intercomparisons (Obs4MIPS) initiative that makes observational data products more accessible for comparisons (Teixera et al., 2014). Obs4MIPS has organised a collection of well-established and documented data sets that have been organized according to the 5^{th} Coupled Model Intercomparison Project (CMIP5) model output requirements and made available through the Earth System Grid Federation (ESGF). The technical alignment of data sets and model output fields is a key element that facilitates the comparison of model data and observations. In addition, Obs4MIPS has created a standardised documentation that is of particular relevance for model evaluation.

The Obs4MIPS activity was initiated by NASA in the US, but there are many opportunities for contributions from a broader community. Broadening of Obs4MIPs to the international community was organised under the umbrella of WDAC by the establishment of a specific Obs4MIPS task team. Ferraro et al. (2015) have summarised the status of the evolution of Obs4MIPs in support of CMIP6. A particular challenge that arises from extending this activity is the management of many more data sets, including multiple data sets for the same model output field and their quality assurance. This calls for a process that allows the provision of information about the quality of data sets included in the Obs4MIPS portfolio. Data set quality assessments, if performed efficiently, could be an attractive activity that provides this information in a systematic way for the full Earth system. Thus, it is important to consolidate standards and high-level practices across WCRP for CDR assessments.

Alongside WCRP activities, space agencies have started a collaborative effort to formulate an architecture for climate monitoring from space (Dowell et al., 2013). This should facilitate the development of an end-to-end system capable of delivering the necessary space-based observations for climate monitoring from space. One of the initial steps was to establish an inventory of CDRs of Essential Climate Variables (ECVs) as defined by the Global Climate Observing System (GCOS). Such an inventory can be used to analyse gaps in this value chain, starting from satellite measurements and ranging to the information provided to decision/policy makers as outlined in the architecture (Dowell et al., 2012). This includes the production and evaluation of CDRs which require a careful assessment of the scientific quality so as not to provide wrong or misleading information downstream. The joint CEOS-CGMS Working Group Climate has started to consider how such quality assessments may be conducted and who could contribute to them. It is obvious that a multitude of differently organised research structures may be able contribute but WCRP leadership through WDAC may be envisaged for this undertaking.

Comprehensive data set quality assessments are critical to move science forward in a systematic way. Trenberth et al. (2014) stated that: "Originally the task was getting a single time series of an ECV. Now there is a proliferation of multiple datasets purporting to be "the correct one". Many are created for specific purposes but all differ, often substantially, and the strengths and weaknesses or assumptions may not be well understood or well stated. Consequently, assessments are required to evaluate these aspects and to help improve the datasets."

In a cycle of quality assessment and reprocessing of data sets, the analysis of data products in direct comparison to reference data, with respect to their consistency with other data sets, e.g., in

representing a part of the energy or water cycle, and/or in comparison with model output data always reveals differences that point to particular weaknesses in certain data sets. More importantly, this can also point to limitations in our capability to perform measurements with the required accuracy and/or sampling. In addition, assessments reveal limitations in our understanding of the measurement process in general, that is, the assignment of traceable uncertainties and our understanding of physical processes that are essential to convert measurements into derived data products. This is particularly true for satellite data sets.

Assessment activities often bring together a critical mass of research groups that analyse deficits and work on improvements of methodology to analyse measurements and the improvement of these measurements, e.g., by defining new satellite missions that address specific deficits in our knowledge.

The following outline for data quality assessments is based partly on experiences gained from the WCRP Core Projects, including the GEWEX Data and Assessments Panel (GDAP; formerly the GEWEX Radiation Panel), described in Kummerow et al. (2012), SPARC and CLIVAR efforts.

3. History of Quality Assessments

GEWEX promotes the assessment of existing data products to adequately characterise each product and its strengths and limitations for various uses. GDAP conducted several data assessments that were related to the establishment of an observations-based estimate of the energy and water cycle over the last decade.

Three quality assessments were finalised: precipitation (Gruber and Levizzani, 2008), radiation fluxes (Raschke et al., 2012), and cloud properties (Stubenrauch et al., 2012, Stubenrauch et al., 2013). Several others are ongoing: aerosol properties, turbulent fluxes over the oceans (SEAFLUX) and land surfaces (LANDFLUX), as well as water vapour. The motivation for these assessments has developed from studying the limits of applicability of a GEWEX data record (precipitation) to real multi-data record comparison exercises (e.g. on radiation, clouds, water vapour, and heat fluxes). All quality assessments were done to determine which data product is best suited to a particular purpose or how a data product could be developed to become applicable in energy and water cycle studies at different space and time scales. Most of the GEWEX assessments that also consider rain gauge data because they are used to calibrate satellite precipitation data records.

Prior to the GEWEX activities, an assessment was performed by SPARC, focusing on upper troposphere/lower stratosphere (UTLS) water vapour (Kley et al., 2000) with the goal of analysing and assessing long-term changes in UTLS water vapour, with an emphasis on the observed increase of water in the stratosphere. SPARC is currently working on an update of this assessment using the improved knowledge and observations from the past 10 years.

The Climate and Ocean: Variability, Predictability and Change (CLIVAR), in particular through the Global Synthesis and Observations Panel (GSOP), has long been promoting and coordinating assessments of various data sets including for example:

- In-situ data sets of sub-surface ocean temperature through the efforts of the International Quality Controlled Ocean Database (IQuOD) [www.iquod.org]. New data sets of sub-surface salinity and oxygen are foreseen,
- Satellite products used for climate studies, such as ocean surface wind, air-sea fluxes (Josey, 2006, Yu et al., 2012, <u>www.oceanheatflux.org</u>)
- Ocean synthesis products, including inter-comparison efforts through the Ocean Reanalysis Intercomparison project (ORA-IP) Joint intercomparison of ocean synthesis & forward model simulation and the EU COST project Evaluating Ocean Syntheses [www.eos-cost.eu].

Members of the CLIVAR community have been actively involved in quality and consistency assessments of ocean vector wind measurements as coordinated by the International Ocean Vector Wind Science Team for ocean surface wind stress measurements from different satellite platforms (Ku-, C-, and L-band scatterometers), and in assessments of satellite measurements of sea surface salinity by the salinity remote sensing community (SMOS, Aquarius, SMAP).

CLIVAR has routinely used these data sets to advance our understanding of the ocean-atmosphere interactions and in particular the role of the ocean. More recently, CLIVAR has established a new research focus on "Consistency between planetary energy balance and ocean heat storage (CONCEPT-HEAT)" aiming to better close the Earth's energy budget. In particular, the CONCEPT-HEAT initiative aims to reconcile different and independent estimates of energy flows derived from independent observing systems, including Argo buoys, in-situ networks, models and satellites, with different sampling capability and accuracy. This innovative initiative will provide new insight into diverse independent data sets related to energy flows, thereby providing scientists with a unique holistic insight.

The assessment activities of the WCRP Core Projects cover only a small fraction of CDRs needed to fully characterise changes in the Earth system but may function as a nucleus for more extensive systematic assessment activities in other domains. Assessment activities have also started in other areas, in particular the oceanic research community. For instance, the International Ocean Colour Coordination Group (IOCCG) sponsored by the Scientific Committee on Oceanic Research (SCOR) and the Global High Resolution Sea Surface Temperature (GHRSST) Climate Data Record Technical Advisory Group, with their associated CEOS so called virtual constellations on Ocean Colour Radiometry and Sea Surface Temperature, have started to develop coordination structures in which data record assessments can be performed.

Discussions among representatives from different communities facilitated by the CEOS-CGMS Working Group Climate revealed many commonalities in current activities, e.g., emerging similar practices of providing estimates of uncertainty, but also important differences, in particular in the specific aims of assessment activities.

4. Assessment Types and Potential Benefits

Data record diversity can be confusing for users and without the proper background information and understanding of the limitations of available data there is a danger that these data may be incorrectly used or misinterpreted. On the other hand, users need to realise that it is often difficult to define a single best CDR. CDRs are instead most often complementary in nature with varying strengths and weaknesses depending on the nature of the application and depending on the observing system used to construct the CDR. For instance, the retrieval of basic cloud properties depends on the sensor channel wavelengths as demonstrated in the cloud assessment of Stubenrauch et al., 2013.

The primary goal of a quality assessment is to highlight differences and limitations of CDRs and, if possible, to justify all aspects of the assessment. Such assessments should become part of the peer-reviewed literature (open access journals preferably) and be distributed as widely as possible, e.g., in ECV inventories, commentary meta-data tools, web portals, etc.

Panels such as GDAP and GSOP currently consider two types of assessments that are valuable to user communities:

 Development of review articles on CDRs considering specific science aspects extending from process understanding to trend analysis, specific geophysical variables (e.g., GCOS ECVs), or topics of importance for IPCC climate assessments. Such review articles could be written by a group of selected experts and reviewed by the panel members not involved in writing the article and journal reviewers. The results can be of immediate use, for instance to IPCC report authors. This also avoids the restrictive approaches on data selection for IPCC reports and provides balanced and peer-reviewed judgement of existing knowledge;

2. Dedicated CDR quality assessment projects that perform a scientific analysis of existing CDRs and publish the results in peer-reviewed literature.

Type 1 assessments may follow cycles of IPCC assessments and can also point to the need for a type 2 assessment, e.g., if the available information for a review article is insufficient and/or incomplete.

Type 2 assessments should not be viewed as static but rather as dynamic activities that are ongoing and provide outputs at regular intervals, e.g., every 2 years. The reporting should contain updates resulting from updated and/or new CDRs, as well as consideration of specific topics, e.g., precipitation in mountainous regions that is hard to observe.

CDR quality assessments are beneficial to science, applications, as well as CDR providers. For the science and user communities, assessments:

- provide independent and transparent quality assurance of CDRs;
- endorse the use and credibility of CDRs for a broader community;
- identify key limitations in CDRs to stimulate improvements;
- allow objective selections of appropriate CDRs,

and for the data record providers the assessments:

- provide background information on available CDRs;
- provide easy access to data in a common user-friendly format;
- establish reference data test-beds and tools for external evaluations that can be reused.

In addition, as many CDRs source data from multiple satellite programmes, the data quality assessments also contribute to an assessment of the strengths and weaknesses of the current observing system. This provides useful guidance on development needs of the future observing system, which is, for example, part of the CEOS-CGMS WG Climate tasks.

5. High Level Best Practices

Generalisation of assessment best practices is sometimes impractical and may not be useful. However, converging on common practices in some areas can ensure a similar level of evaluation of the quality of CDRs. These records may cover various aspects of the Earth climate system and may include many types of measurements (ground-based, satellite-based, in-situ and derived products that may combine measurements from multiple sources) as well as data from reanalyses. To make assessments comparable it is important to agree on some high level principles:

- 1. While assessments should include the creators of the CDRs being assessed, the assessment team needs to extend well beyond that group so as to avoid data products being evaluated favourably by the developers to encourage data use;
- 2. Assessments need to target well-developed expectations of CDRs such as those documented in GCOS-143 or those encapsulated in the GCOS Climate Monitoring Principles. By ensuring that each assessment targets these key requirements on CDRs, each assessment will have a similar structure and the user community will develop clear expectations of what assessments will encompass. However, the structure should not be so restrictive as to prevent the publication of results unique to the assessment. Every assessment must, at the very least, document the scientific utility of the CDR being assessed as well as the characterisation of uncertainties in the CDR;
- 3. A lexicon of best practices to create CDRs also including practices on data comparisons and nomenclature used for characterising uncertainties;
- 4. Metrics to assess how far best practices have been followed.

These four principles should be adhered to any group performing an assessment.

1. Under general procedures, it is understood that each assessment should be hosted by a scientific body to whom the group performing the assessment reports, and who would be responsible for the assessment report. As mentioned above, the assessment is tasked to conduct objective and independent evaluations and inter-comparisons. It is advantageous to involve the scientists that created the CDRs so that sufficient background information on the instruments providing the measurements, applied methods, and underlying assumptions and limitations can be captured in detail and conveyed to the user. However, to ensure independence, independent experts need to be included in the assessment team to prevent biases in the reporting of results for specific CDRs, e.g., by selection of a particular comparison metric, reference data, or physical range of parameters. Although this is not easy, various groups have achieved such level of independence through various processes, such as reporting to a governing panel/project or via external review.

Another aspect of involving product developers in an assessment is the tendency to broaden the goal of the assessment from its original intent of informing the user community, to one of using the assessment itself as a diagnostic to help investigators improve their respective data products. Although this is a clear benefit for the data producers and may ensure their participation, it has been found that while these two objectives are compatible, they should always be kept distinct in the assessment so as to keep the assessment manageable. Thus, in general, a data quality assessment should concentrate on providing information to the science and user community first, and then move to updates of the various data sets considered outside of the assessment.

- 2. As a general structure, an assessment of climate data records should always cover the following elements:
 - A survey of available CDRs with their related background information;
 - A quantitative comparison against reference data (especially if data of higher accuracy and/or maturity are available), if available, to elucidate the strengths and weaknesses of the CDRs being assessed;
 - Comparisons of different CDRs at different temporal and spatial scales. GDAP has found that including model and reanalyses data sets in the comparisons is often useful in that it immediately incorporates the needs of an eventual user community;
 - Recommendations for intended CDR uses and identification of areas for which data should not be applied;
 - Open, full, and easy access to the assessment report and all examined CDRs¹ and methods.

With regard to the last item, it has been found that even if the validation data, procedures, and previously assessed data are archived for interim use, comprehensive assessments are critical to move the field forward in a systematic way.

Furthermore assessments should include:

- A dedicated, motivated, and respected expert or group of experts to lead the effort;
- Assessment team members with individual, but complementary, specialized knowledge;
- Regular team meetings open and closed workshops;

¹ Some data will not be hosted in one place because of high data volumes. Thus, easy access is fulfilled if the data are readily accessible via internet without needing special permission.

- A centralized data repository created specifically for the assessment (e.g., validation data or common gridded products) that can be used to facilitate assessments with new products or new versions of existing products.
- 3. A charter of best practices to ensure coherent use of nomenclature should be developed and hosted by a sub-group of WDAC. Such a lexicon would need to be coordinated with other bodies such as GCOS and the CEOS-CGMS Working Group Climate. Such a development could benefit from on-going initiatives such as QA4EO and related projects such as the European QA4ECV project.
- 4. A procedure to assess the extent to which best practices have been followed in generating the CDRs is useful in the survey of available CDRs and also helps to keep the assessment activity manageable by concentrating on CDRs of a certain maturity. Progress on such metrics, for example based on the work published by Bates and Privette (2012), has been made in projects such as the European Union project CORE-CLIMAX (CORE-CLIMAX, 2015).

In addition to the described best practices, each assessment needs to have a strategy for the dissemination of its results and how to make an impact on the scientific community. The classical way of peer-reviewed publications and a WCRP report remains important because it ensures a proper review. However, the WCRP core project web appearance should put stronger emphasis on assessment activities and results. Data catalogues from data providers could be enhanced with tools providing commentary meta-data for a data set, e.g., those developed in the EU CHARMe project. These can point to assessment results and also databases used in the assessment. In addition, the Obs4MIPS platform can also serve as a good means to disseminate the results, at least for those data sets of potential use in climate model evaluation. Finally, other suitable online platforms such as the NCAR Climate Data Guide can be used for better dissemination to the community.

6. Support Needs

Past and current assessment activities usually relied on pure voluntary efforts, and thus can take considerable time to finish and can even collapse without strong leadership. Within GDAP several assessments took a very long time (>10 years), a timespan far too long to address the needs of such assessments. Full funding of assessment activities is out of the scope of most funding agencies, however, ideally some seed funding for centralized activities, e.g., on a centralised data depot and initial workshops should be provided to establish the assessment. A good recent example is the setup of the GEWEX water vapour assessment, for which ESA sponsored an initial workshop and EUMETSAT is funding central activities for about two years through its Climate Monitoring Satellite Application Facility (CM SAF). This allows the assessment to advance and keeps the participants together and active.

It is recognised that funding practices strongly differ across the globe but the membership of WDAC, including the CEOS-CGMS WG Climate (representing space agencies), can certainly help to improve the situation if convincing cases for assessments are brought forward. Such cases could be taken up by existing national and international programs, such as the NOAA Climate Data Record Programme, NASA Measures, ESA Climate Change Initiative, EUMETSAT SAFs, and other initiatives.

7. Governance Aspects

A couple of relevant questions related to the governance of assessments are:

- Who should initiate an assessment?
- Who should organise it?
- Who should undertake the assessment?
- Who should evaluate quality assessments?

Currently, there is no overall coordination of data record quality assessments related to GCOS ECVs; energy, water, and matter cycles; or other topics of importance to the IPCC. Assessments are often initiated and performed by specific scientific or other organisational bodies that represent both users and developers. The aims of these assessments range from providing objective information to the scientific community about the status of data records to more ambitious goals such as making trend estimates and using the data record comparison as a means to find or create the best data record for a specific purpose. Data record assessments are much more common in communities and bodies that work with satellite data compared to those related to in situ data records.

It is suggested to initiate data record quality assessments by any scientific or organisational body that identifies a need for such an assessment. However, the assessment then needs a 'harbour in which to anchor', to ensure support and an independent review.

Within WCRP the Core Projects may task relevant panels or groups of experts to act as initiator, organiser, and reviewer of data record quality assessments following the model set out here For assessments requested from outside, e.g. from the CEOS-CGMS Working Group Climate, WCRP should play a critical role in performing them; WDAC could become the known receiver of such requests and can help to channel it within WCRP. WDAC could also play an important role for developing a prioritisation of assessment needs to guide funding agencies in their support of assessments.

The organisation of an assessment is best placed at the level of panels or activities within WCRP core projects, because this is the place where scientific knowledge is concentrated and lead scientists for assessments can most easily be identified.

Scientific groups undertaking assessments should be formed in an open way to assure broad participation, however, attention should be paid to the selection of data records so as not to end up with only once-off activities that are of limited value to users. The scientists leading the assessment need to report to the group overseeing the particular activity/panel at regular intervals, e.g., annually. This group, for example a core project's Scientific Steering Group (SSG) would then report to the WCRP Joint Steering Committee (JSC).

Organisation of assessments will not be restricted to WCRP since other domain/topic-specific bodies (e.g., CGMS working groups as ITWG, IPWG, CEOS Virtual Constellations) exist that may organise their own assessments.

The role of WDAC should be to oversee assessments performed within and outside of WCRP, in particular pointing out where assessments potentially lack in critical areas for science, the IPCC, and climate services. The WDAC membership is ideally positioned to do this in coordination with GCOS and the space sector. WDAC could establish an inventory of assessments that could be provided to various bodies such as the WCRP JSC.

By identifying area where assessments are lacking, WDAC can also act as the initiator of data quality assessments, which may, at a later stage, be performed by WCRP core projects. WDAC should also be active in supporting the funding of data quality assessments since this is vital to ensure the success of these assessments. In addition, WDAC could organise the collection and publication of best practices for climate data record generation.

8. Conclusion

This document provides an outline for data quality assessments explaining the needs, benefits, high level best practices, and a potential light governance structure. It is mostly based on experiences from the GEWEX Data and Assessments Panel, but also refers to more recent discussions among space agencies on the architecture for climate monitoring from space where quality assurance is a very important topic.

WDAC is invited to take note, discuss, provide feedback, and lay out a way forward.

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10. Glossary

CEOS	Committee on Earth Observation Satellites
CGMS	Coordination Group of Meteorological Satellites
CHARMe	European Union Framework 7 Project on commentary metadata and tools
	(charme.org.uk)
CLIVAR	Climate and Ocean: Variability, Predictability and Change (core project of WCRP)
CMIP	Coupled Model Intercomparison Project
CM SAF	EUMETSAT Satellite Application Facility on Climate Monitoring
CORE-CLIMAX	European Union Framework 7 Project in the context of Climate Services
	(<u>www.coreclimax.eu</u>)
ECV	Essential Climate Variable (defined by GCOS)
ESA	European Space Agency
ESGF	Earth System Grid Federation
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GCOS	Global Climate Observing System
GDAP	GEWEX Data and Assessment Panel (former GEWEX Radiation Panel)
GEWEX	Global Energy and Water Cycle Exchanges (core project of WCRP)
GHRSST	Global High Resolution Seas Surface Temperature (international open group for
	SST data producers, users, and scientists)
GSOP	Global Synthesis and Observations Panel (CLIVAR panel)
IOCCG	International Ocean Colour Coordination Group (affiliated programme of SCOR)
IPWG	CGMS International Precipitation Working Group
IPCC	Intergovernmental Panel on Climate Change
ITWG	CGMS International TOVS (TIROS Operational Vertical Sounder) Working Group
JSC	Joint Scientific Committee (highest scientific body of WCRP)
LANDFLUX	GDAP project on turbulent heat fluxes over land surfaces
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPS	Observations for Model Intercomparisons
QA4EO	Quality assurance framework for earth observation (QA4EO has been endorsed by CEOS as a contribution to facilitate the GEO vision for a Global Earth Observation System of Systems (GEOSS).
QA4ECV	European Union Framework 7 Research project on establishing a Quality
QA4LCV	Assurance Framework for Climate Data Records (www.qa4ecv.eu)
SCOR	Scientific Committee on Oceanic Research
SEAFLUX	GDAP project for turbulent heat fluxes over ocean
SPARC	Stratospheric-tropospheric Processes and their Role in Climate (core project of
JFARC	WCRP)
SSG	Scientific Steering Group (sub body of WCRP core projects that reports to the WCRP JSC)
UTLS	Upper Troposphere Lower Stratosphere
WCRP	World Climate Research Programme
WDAC	WCRP Data Advisory Council