Quality Assurance as seen from the database

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This document, which was prepared in fulfilment of Deliverable 6.3 in the EDUCE project, attempts to explain and recommend to data submitters, database users, and database managers and operators the nature of Quality Assurance as seen from the database point of view, and the consequent implications for the methods adopted at the observing sites and at the database when carrying out Quality Control procedures and preparing the resulting data and ancillary information for presentation to the potential users of the database.

The first section below describes the distinction between Quality Control and Quality Assurance for our present purpose, and sets out the general philosophy of our approach. The second section reviews the nature of Quality Control as performed at the observing sites, with the ultimate goal of Quality Assurance in mind, and the third section describes the nature of the relevant evidence that is conducive to achieving some degree of Quality Assurance at the database. Finally, the fourth section looks to the future and considers the desirable goals for Quality Assurance in a database of this type.

1. Quality Management

The term Quality Management encompasses the various tasks that are encountered as soon as quality is to be regarded as an important attribute of a product, an attribute that merits examination and description. Quality Management therefore includes Quality Control and Quality Assurance, as well as other tasks that are found in some commercial and advanced applications, such as Quality Improvement. In the EDUCE project we are interested only in Quality Control and Quality Assurance, so we begin by describing the meaning of these terms, at least for the narrow purposes of this document, which is concerned only with the application of Quality Management to the development of the EDUCE database.

Quality Control

Quality Control is essentially the process that monitors the quality of the product and takes some appropriate action in those cases where the quality falls short of the expected level. It follows that a certain level of quality is expected, and that the operators know what that level is. They must also have the means to assess the quality of the product, either by examining every item or by taking samples for examination or by some other means such as monitoring statistics from the production process. In practice a combination of techniques may be used to assess various attributes of the quality. If the quality falls short of the required level, the Quality Control system will have a procedure for invoking corrective action. This may take the form of rejecting defective items, or adjusting the machinery to produce a better quality, or giving the staff a break, or altering some other part of the production process, or carrying out an investigation to arrive at a solution to the problem.

In the case of ultraviolet spectroradiometry, Quality Control is the system of procedures that are designed to establish the quality of the measurement results. These procedures include tests such as calibrations that provide or enhance the inherent quality of the measurements, as well as monitoring tests that assess their quality by examining the measurement process retrospectively.

Throughout the process of Quality Control it is clear that good documentation is required in order to keep track of the tests, but if it were only for Quality Control the documentation could be in a form which was available only to the local operators, and it would be sufficient if it could be understood by all those involved in the Quality Control system. The documentation would not have to leave the site, and it might be thought that it could even be destroyed after a while, having served its purpose of achieving a satisfactory level of quality. Of course, even in commercial and industrial production the documentation arising from the Quality Control process is likely to be of value long after the event, as it may reveal incipient faults in the equipment, or enable a faulty batch to be traced to a particular machine or operator. In ultraviolet spectroradiometry the Quality Control documentation is also likely to be of use in the retrospective diagnosis of instrumental problems, and in any case it is useful to have a record of past performance as a guide to the effectiveness of current and future procedures. For these and similar reasons it is usual for Quality Control documentation to be retained long after it has lost its immediate relevance, even if it has become intelligible only to those with very long and local memories.

But there is a much more compelling reason to retain the documentation from the Quality Control system, and to record it in a form that can be understood by the external reader. That reason is Quality Assurance.

Quality Assurance

Quality Assurance is the process that seeks to convince the customer that a certain level of quality has actually been achieved. The customer will only be persuaded by hard evidence in a form that can be examined in detail, just as a financial auditor will only be persuaded by a complete set of accounts. The regularity and tidiness of the evidence are just as important in Quality Assurance as they are in accounting. In the commercial and industrial sectors the principal evidence in favour of Quality Assurance will come from the records of the Quality Control processes, so it is essential that these are carefully documented. Additional evidence comes from independent assessment of the Quality Control system. From the customer’s point of view, this type of evidence is particularly compelling, as it does not depend solely or even directly on the machinations of those who made the product. In the real world of manufacturing and commercial services, Quality Assurance is successful only to the extent that the Quality Assurance inspector is thorough and incisive in evaluating the design and performance of the Quality Control system. The Quality Assurance system has succeeded if the customers feel that they would have reached the same assessment of the quality even if they had been present as active assessors throughout all stages of the production process.

It follows that in ultraviolet spectroradiometry the aim of Quality Assurance is to convince the user of the database that the measurements live up to a certain level of quality. It may be the level expected by the user, or the level required for a particular purpose, or the level stated in a document associated with the data. In any case, Quality Assurance aims to demonstrate what level of quality has probably been achieved.

The role of Quality Assurance in ultraviolet spectroradiometry is therefore rather more general than in commercial and industrial applications, in that it aims to set the quality of the data in context against a range of possible levels, reflecting the needs of the users.

Some data users will be content with a minimal level of quality because they require only a rough estimate of the radiation quantities, whereas others will need to be satisfied that a high level of quality has been achieved, for instance because they intend to draw quantitative comparisons with data from other sources and only measurements of high absolute accuracy will serve their purpose.

Moreover, the quality of the data will vary greatly from one measurement to another, and from one recorded spectrum to another, according to the solar zenith angle, the wavelength, and other parameters. For some applications all these data will be appropriate and useful, while other applications will call for a careful selection of suitable cases.

Ideally, therefore, the Quality Assurance system in ultraviolet spectroradiometry will enable the database user to assess the quality of the data, rather than merely to confirm that it meets a prescribed level.

2. Relevance of Quality Control (QC) procedures to Quality Assurance (QA)

In principle, Quality Assurance consists largely in demonstrating that the Quality Control system has operated correctly, so the various parts of the QC system can each have an influence on the outcome of the QA process. However, this relationship between QC and QA applies strictly to the fully specified and documented procedures encountered in quality management systems that have been formally certificated by approved accreditation bodies. In ultraviolet spectroradiometry the quality management systems are generally uncertificated and the specification of the individual procedures is less formally prescribed and documented. Consequently, in these systems, not all aspects of Quality Control will lend themselves to the requirements of Quality Assurance. Nevertheless, within the EDUCE project, most QC procedures have the potential to contribute to QA, but only to the extent that they can be seen by the data user. The relevant QC procedures fall mainly into two categories, which we can broadly describe as internal and external.

Internal QC procedures are those that are performed routinely by the operators at the observing sites in order to control and establish the calibration and performance of the spectroradiometers. The relevance of these procedures to QA depends on the extent to which they can convince the user that the measurements are accurate enough, particularly as regards those characteristics which are difficult or impossible to check by any other method. In this respect the most critical factors are those that affect the absolute irradiance calibration, the location, date and time of observation, and the angular response of the receiver. Other factors such as the slit function and the wavelength calibration are lower in priority, not because they are irrelevant to QA but because their effect on the quality of the measurements is more readily accepted without corroborating evidence from the QC system.

The wavelength calibration is one of the factors that is least dependent on thorough QC procedures, simply because the evidence for it is contained mainly in the results themselves, rather than in the supporting documentation. Consequently, the critical user is much more likely to assess the accuracy of the wavelength calibration by carrying out an analysis of the spectral irradiance data than by studying the internal reports of wavelength checks based on spectral discharge lamps. However, there are three remarks that might be made in qualification of that general statement. Firstly, the operators can themselves carry out such a data analysis as part of the QC procedures, in which case the user may choose to rely on it. Secondly, the most exacting requirements for accurate wavelength calibration will actually require detailed laboratory calibration against spectral discharge lamps or lasers, as primary sources of wavelength information, rather than relying solely on published details of solar extraterrestrial spectral structure. And thirdly, the wavelength scale of the absolute spectral irradiance calibration cannot be found by examining the irradiance data, but must be supported by adequate information from the internal QC procedures to show that the wavelength calibration did not alter significantly between the laboratory irradiance calibration and the subsequent solar irradiance measurements.

In the case of the slit function a single determination tends to speak for itself, not only as to the width and shape of the function but also as to the quality and reliability of the determination. The user can see the extent of the detail and can judge whether the measurement was limited by the nature of the light source. The relevance of slit function determinations to QA therefore lies in (a) the extent to which they reveal the slit function itself in full detail, (b) the repeatability of the slit function characteristics during a series of determinations and over a long period of measurements, and (c) the variation in the slit function across the spectral range of the instrument.

In contrast to the wavelength calibration and the slit function, the factors where QC procedures are most critical to the achievement of QA centre on the absolute irradiance calibration, the location, date and time of observation, and the angular response of the receiver. The last of these, which usually consists of the cosine response of the diffuser or integrating sphere determined at four rectangular azimuths, is one of the most difficult aspects of QC to present in a form suitable for QA purposes. The experiment is awkward to set up and control, and usually rather tedious and time-consuming to execute, so the user is often presented with only one determination, which must stand for years of solar irradiance measurements. Moreover, the effect of the angular response on the actual results can depend rather critically on the methods used to incorporate information on the azimuthal variation, and the distribution of radiance around the sky. This is a case where the QC procedures can have a profound effect on QA, as everything turns on the skill with which the operators communicate their care and competence to the data user. The aim of the relevant QC procedures is to establish the angular response in sufficient detail to allow adequate correction of the spectral irradiance measurements, and therefore to show that its repeatability, and its variations with wavelength and the passage of time, have been sufficiently examined and determined.

By contrast, the location, date and time of observation are relatively straightforward to deal with, but they are nevertheless vital, as a spectral irradiance measurement is worse than useless if these labels are wrongly recorded. The QC procedures that ensure accurate timekeeping and correct labelling are therefore an important part of subsequent QA. A data user who can see carelessness or incompetence at this level is not likely to be convinced that the laboratory calibrations got the attention they deserved.

The measurement process itself also deserves attention within the QC system, as the quality of the measurements depends on attention to details such as the duration of the spectral scan, the wavelength step, the treatment of dark current and stray light, temperature stability, the levelling of the receiver, and the position of obstacles in the field of view.

Finally, we come to the most important and yet the most difficult of the internal QC procedures: the absolute spectral irradiance calibration. There is no need to dwell on its relevance to QA: suffice it to say that a deficient irradiance calibration makes all the rest of the QC procedures rather pointless. Every detail of the spectral irradiance calibration is therefore capable of contributing to QA, and the absence of any step automatically detracts from QA. These details range from the fundamental standard to the final instrument calibration, and therefore include the quality of the calibrations attached to the lamps obtained from the national standards laboratory, their consistency and constancy over a period of time, the repeatability and stability of the calibrations of transfer standard lamps and their mutual agreement, the experimental arrangements for the spectral scanning of lamps by the spectroradiometers, and the behaviour of the resulting instrumental calibrations during each experimental determination and over the period during which solar irradiance measurements have been recorded. If these matters are to contribute to QA, the user must somehow be convinced that each detail has been properly taken into account in the QC procedures, and that nothing has been forgotten or neglected. All this has to be achieved at a distance, as the database user does not generally have the opportunity to inspect the processes at the observing site – not even after they have long ago been completed, far less while they are actually taking place. As critical examples of this, consider the following two cases. In the first case, the distance from the spectral irradiance lamp to the instrument receiver is measured and set at the nominal distance, typically 500 mm or 700 mm, but the distance is measured from the wrong plane in relation to the lamp housing, thereby departing from the conditions under which the lamp calibration was originally determined. How is the database user to know? In the second case, the walls of the calibration room are painted matt black, but the rails of the optical bench are bright metal and reflect extraneous light from the lamp on to the instrument, thereby corrupting its calibration, as demonstrated by subsequently placing a black cloth over the offending rails. Both cases have been encountered in practice. If the operators do not realise that there is a problem, how can the QC procedures provide the necessary contribution to the QA process? The next section will provide one possible answer to this conundrum, and we shall also return to it later when considering evidence conducive to QA at the database.

In addition to the internal QC procedures which are carried out routinely by the operators at the observing sites, there may also be external QC procedures. These are of two main types, both aimed at throwing further light on the calibration and performance of the spectroradiometers. The first type is the instrument intercomparison campaign, in which a number of spectroradiometers are brought together at one place to measure the same irradiance spectrum simultaneously. The second type is the peripatetic audit inspection in which an independent operator examines and assesses the operating conditions and procedures at the observing site. The audit inspection may also include a travelling spectroradiometer which can be used to provide a standard against which to compare the local instrument. In both these types of external QC, the advantage is that the procedures are carried out independently of the local operators, and therefore provide information which is of additional value as a contribution to the QA system. An external audit may reveal details of the calibration and measurement processes that were previously overlooked, while an instrument intercomparison offers an alternative view of the calibration, which automatically incorporates all the intermediate steps and influences, assuming that the calibration of the travelling instrument is accurate. This provides a check on any factors that have been overlooked in the local calibration procedure.

We have discussed the various internal and external QC procedures and their relative importance from the point of view of the QA system, but in ultraviolet spectroradiometry most QC procedures are not carried out with QA in mind. It is therefore now necessary to consider what evidence can be gleaned from the QC system that might contribute to Quality Assurance for the database user.

3. Evidence conducive to Quality Assurance at the database

From the database point of view, the evidence for QA is perceived first by the database manager and then by the database user. Both are to be persuaded by the results from the QC system that the data satisfy four desirable criteria, each relative to whatever purpose the user might have in mind. These criteria are availability, suitability, reliability, and accuracy.

Availability

The first criterion derives its evidence directly from the spatial and temporal information in the database, which depends on the QC procedures that record the locations, dates and times of the observations. Quality Assurance begins at this point, as any confusion or inconsistency in the names of the sites will sap the user's confidence at the outset, and the data are much less likely to be used if the availability of observations is sparse or patchy. For many purposes the first requirement is that the recorded spectra should be continuously available at regular intervals over an extended period. Paradoxically, therefore, availability can sometimes be the most crucial aspect of QA. Whenever possible, data providers should strive to record a complete set of spectra on a regular schedule for a period long enough to represent climatological conditions.

Suitability

If observations are available at the date and place selected, the next requirement is that the spectra should be suitable for the purpose in hand. In most cases this turns on the range of wavelengths recorded, and to a lesser extent on the wavelength resolution. As ultraviolet spectroradiometry is generally aimed at studying either atmospheric photochemistry or biological effects of radiation, the spectral data must cover the range of wavelengths that are important for the relevant photochemical or photobiological process. It is therefore important that data providers should attempt to offer spectra covering the wavelength range of the action spectra that are likely to be employed by the users.

Reliability

Now we come to a more critical aspect of QA at the database. This is currently the stage at which the user of the EDUCE database is most likely to judge the quality of the data on the basis of the evidence that is visible in the database. Quality Assurance derives from the user's confidence, which is invariably enhanced by the sight of professional competence and methodical care. As the fine details of the QC procedures at the observing sites are largely hidden from the user at present, the quality of the resulting data is likely to be judged by the appearance of the records held in the database. These records range from the station names to the spectral irradiances, and can be assessed on the basis of their regularity and consistency. High quality data will be free from any confusing duplications, gaps, and ambiguities. For example, the station identifiers will be unique to each distinct observing location; the data will cover an extended period of many months or years with few if any missing days; the observations will cover the hours of daylight from near dawn to near dusk at regular intervals of not more than an hour; the wavelengths will cover a consistent spectral range at a constant wavelength step; and the irradiances will be in the range expected for the location, date and time.

Accuracy

This is the most difficult criterion for the QA system to satisfy. The user can only be convinced that a certain level of accuracy has been achieved by making use of all the information available, at the database and elsewhere. Apart from any procedures available at the database to check compatibility of the spectra with externally specified wavelength and irradiance scales, the user must judge the quality of the data by careful examination of the QC documentation from the observing site or by attempting to carry out quantitative tests on the plausibility, internal consistency and validity of the spectral irradiance data. As such quantitative tests are nearly impossible to carry out in practice, and likely to produce inconclusive results, most users will resort to the only other readily available source of information, namely the results of instrument intercomparisons. Whether these are from grand international campaigns or local comparisons with a travelling standard, they have the merit of providing an independent assessment of the measurement accuracy, and suffer only from the relatively minor objections that the comparison standards are not perfect and that the instrument calibration may drift after the comparison. Perhaps their greatest advantage is that they automatically incorporate the effects of any sources of error that were overlooked in the local calibration and measurement procedures.

As the most useful sources of information on accuracy are the QC procedures and the results of intercomparisons, the documentation of these sources must be made available to the database user. The results of the grand international campaigns are generally available as technical reports, and the same should be true for the other external QC procedures such as independent audit inspections and comparisons with travelling standards. As for the internal QC procedures, it is up to the operators to make the results available to the database users in a form which will enable them to assess the accuracy of the measurements. Clearly, that can only be done if the same information is made available as was used by the operators in arriving at their own assessment of accuracy. It is to be hoped that in the fullness of time such information becomes available in a standard form so that the assessment is straightforward and comparable at different stations.

4. Further progress in Quality Assurance

In ultraviolet spectroradiometry, the future of QA depends largely on the development of adequate procedures to establish the accuracy of the absolute spectral irradiance calibration. In order to provide a uniform method of assessment, the accuracy of the irradiance measurements will be evaluated in terms of uncertainty, using the existing QC procedures to provide the estimates for each component of uncertainty. Ideally, provision will be made for any number of estimates to be carried out, so that the uncertainty analysis can be made independently, and can be improved as new information becomes available or a more thorough treatment becomes possible. It should be possible to reconcile the uncertainty estimates based on internal and external QC procedures, and thereby obtain a combined estimate, and it will be necessary to enable the calculation of the uncertainty parameters for each individual measurement, as they will clearly depend on the solar zenith angle, the wavelength, and other observing conditions. Finally, it must be possible to store the requisite uncertainty information in the database to accompany the measurements, and to propagate the calculated uncertainties appropriately to any data products that depend on the spectral irradiance measurements.

Throughout the development of Quality Assurance systems, the aim is to convince the user that a certain level of quality has actually been achieved, so it is essential that the method of arriving at uncertainty estimates, and other steps in the quality management system, are described in full detail, so that the user can assess the implementation of the quality systems and judge whether the level of quality achieved is likely to be adequate for the purpose in hand. These considerations are as relevant to the current quality management systems as they will be to those of the future.