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Digitization versus Digitalization & Digital Transformation in the field of calibrations and their subsequent use

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1 Abstract

Digital transformation activities have been carried out in the field of calibration since 2017, in particularly with the digital calibration certificates (DCCs). From the very beginning, these activities have been designed to cover the entire field of calibration, from NMI to production and across national borders. This philosophy of considering the requirements of all the parties concerned has shaped the history and the roadmap of the DCC, which are described in section 2. At the third international DCC conference, which took place from February 28 to March 2, 2023, and attracted great interest from the community, one of the topics was "DCC and Digitization vs. Digitization & Digital Transformation". This topic will be treated in section 3. As can be seen, the difference between the development step of “DCC & digitization” and the development step of “digitalization & digital transformation” is significant. The benefit that is assumed to arise for the economy as a whole by means of the “digitalization & digital transformation” step is a clear reason in favour of it. An analysis of the presentations held at the third DCC conference confirms this assumption. In this paper, we will show the advantage such a course of action will bring about. In section 4, we will compare the IT technologies that are preferred to achieve the aim of the digital transformation. XML will be contrasted with PDF/A3 and the advantages and disadvantages of both will be discussed.

Keywords: DCC, Digital Calibration Certificate, Calibration Report, Calibration, SI, D-SI, XML, PDF/A3, Digital Signature, Quality Infrastructure

2 Description of the PTB-coordinated DCC

2.1 History

The DCC project described in this article is coordinated by PTB. Many suggestions and proposals from the international community regarding calibrators and calibration users have been included in the DCC. The DCC has already been presented in numerous publications, meetings, and workshops. The DCC is a project geared towards the international community. This depends on the feedback and cooperation of a wide range of international partners (i.e., from industry, from calibration laboratories and from the NMIs) and on their cooperation.

Scientifically, the development of the DCC started in 2017 with the first publication on this topic [1]. A chronology of the topics of the publications dealing with the development of the PTB-coordinated DCC as well as of other publications about the DCC is shown in Table 1.

The DCC [45] has a website of its own for some time now where you can find all the information needed to become familiar with the topic. Apart from a Wiki [46] on the DCC, more additional and important information can be retrieved there, for example examples of Good Practice (GP) or information about the GEMIMEG tool [47].

The BIPM website [48] points out the importance of digitalisation, see "Joint Statement of Intent - On the digital transformation in the international scientific and quality infrastructure" [49], which has been signed by many other organisations besides the BIPM.

Table 1: Publications directly on the DCC

Year	Publications
2017	[1], [2], [3], [4]
2018	[5], [6]
2019	[7], [8]
2020	[9], [10], [11], [12], [13], [14], [15], [16], [17], [18]
2021	[19], [20], [21], [22], [23], [24], [25], [26], [27], [28], [29]
2022	[30], [31], [32], [33], [34], [35], [36], [37], [38], [39], [40], [41]
2023	In addition to the conference volume of the third international DCC conference [42], with 1146 registrations from 93 countries and 56 presentations, the publications [43], [44] were released in 2023.

2.2 Short description of the PTB-coordinated DCC

DCC makes it possible to digitally transform calibration reports based on ISO/IEC 17025 [50]. The data are transformed into a data format that is suitable for long-term storage and has a structure that is available free of charge with an open-source license.

2.2.1 Coordination and transfer

Due to intensive communication within the DCC community, the DCC is continuously being further developed, e.g. by means of international DCC conferences [34], [42]. Furthermore, there is a series of activities undertaken by various committees such as the *Deutscher Kalibrierdienst* (DKD [51], [52]) (German Calibration Service) and close cooperation with accreditation bodies, especially with the *Deutsche Akkreditierungsstelle* (DAkkS [53]).

Apart from the NMIs and DIs, it is especially the calibration laboratories, the accreditation bodies and the end users of a calibration which are part of the DCC community.

In June 2022, a summer school was organized, whose aim it was to support the coordination of the DCC and the transfer of knowledge about it. Two groups of approximately 40 participants each were trained for two weeks. The international participation enabled a worldwide transfer of ideas and know-how around the DCC.

License

The concept of the DCC is such that no license costs will occur for its use. In the terms of license of the XML scheme it says: “This XML Scheme Definition (XSD) is free software: you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation, Version 3 of the License.”

Internationality

The DCC is geared to users worldwide and is not focused on a single company or a single community. On the contrary, it is geared to all levels of the calibration pyramid:

- from the NMIs, which are at the top of the pyramid in their respective countries, exist all over the world and are excellently connected with each other in networks,
- via the accredited calibration labs,
- the in-factory calibration labs,
- the calibration labs (production),
- to the products and services,
- the DCC has a broad range of application.

The DCC will be disseminated worldwide due to the fact that the NMIs and DIs are embedded in networks and as such will ensure that the national standards are compared in key comparisons (this is shown in Figure 1 on the left-hand side). Key comparison" is synonymous with the terms "interlaboratory comparison" and "ring comparison". We use the term "key comparison" in this publication. In the graphic representation on the right, the concept of the calibration pyramid is shown schematically.

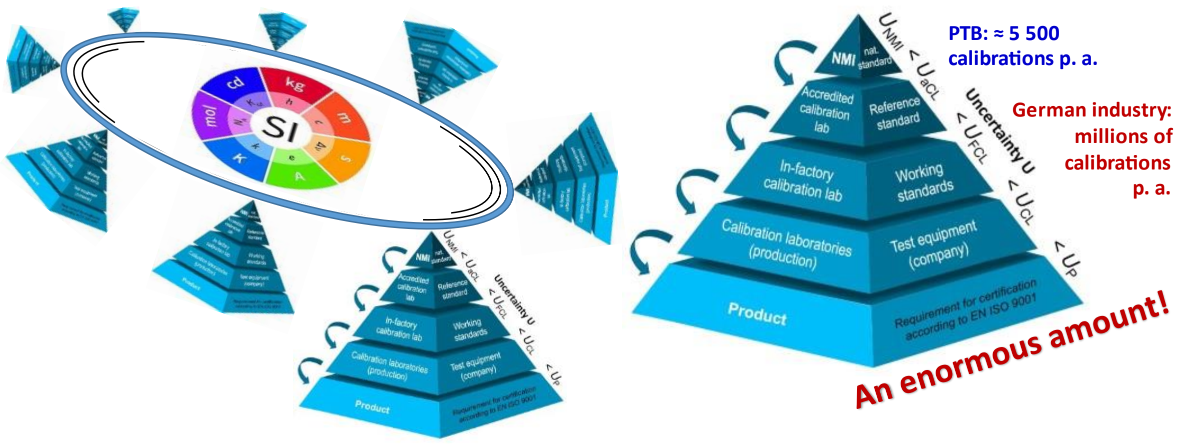

Figure 1: (left) Key comparison (schematic representation), (right) calibration pyramid.

At PTB, for example, approximately 5,500 calibrations are carried out per year. In contrast to this, some of the large, accredited calibration laboratories (and there are many of these!) carry out 3,000 calibrations on one single day! This makes it clear that from the top of the pyramid to the second level, there is an enormous multiplier effect. It also underlines the influence a reliable and authentically transferred calibration certificate has on production which, in addition, is entirely machine-interpretable.

2.2.2 Macroeconomic aspects of the DCC

In a paper from the World Bank dated 2007 [54], Guasch et. al. pointed out which significance a national quality infrastructure has for the national economy of a country (Figure 2).

Just what an important role calibration certificates play becomes obvious from Figure 2. The fact that it is ensured that calibration results are transferred in a faultless, integer and authentic way has a direct effect on a national economy. For this reason alone, it is important to pay close attention to these aspects when performing the digital transfer from the analog calibration certificate to the DCC.

The benefit of the DCC for industry and, in particular, for a national economy lies in the fact that it offers the possibility to significantly improve the total quality management (TQM [55]) due to accurate measurements. Some of the keywords here are the saving of resources to protect the environment, and the potential of CO_2 reduction. At the same time, the quality of the products is significantly improved because faults during the transfer of data are ruled out and high-quality, trustworthy data can be provided.

As we are currently in the era of the 4th Industrial Revolution, there are further aspects to be taken into consideration:

- The data of the DCC must be made usable for modern production methods.
- The data must be made machine-interpretable (see section 3).
- It must be possible to choose a data format that ideally meets the needs of the partners in the calibration pyramid (see section 4).
- The FAIR principles [56] (see also 4.3 below) must be observed.

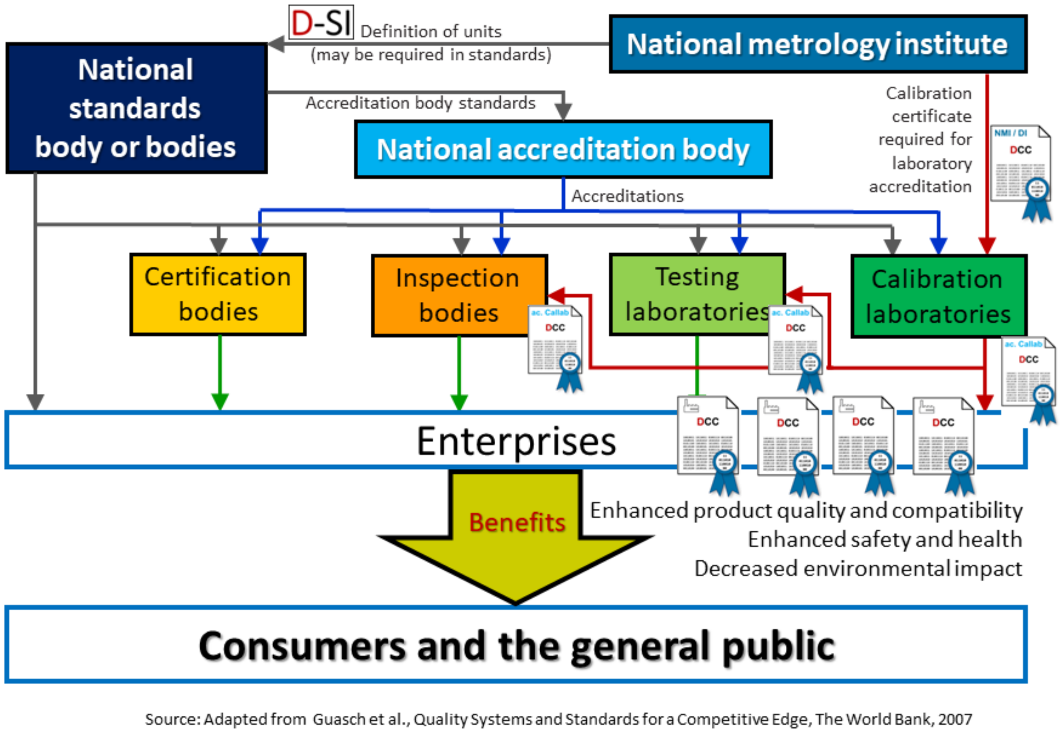

Figure 2: Representation of a national quality infrastructure (based on [54])

As far as the costs for industry are concerned, the following question will certainly arise: How long will it take until the investments made into the DCC will have amortized (which is known as *return of invest* - ROI)? Or, more generally: Which processes can contribute to optimizing production by using the DCC? The following advantages are obvious here:

- An increase in quality because faults are prevented
- The reduction of faulty products
- The re-use of calibration data, also in other applications
- The adjustment of the calibration intervals to the identified needs
- Independence from a calibration laboratory
- The automated transfer of calibration data into content management systems is possible, i.e., the four-eyes principle is no longer necessary.
- The automated transfer of calibration data into production machines (fault avoidance and fault reduction) without having to change between different media.
- Protecting the environment and saving resources by using a paperless digital format.

2.2.3 Company interests

Every company that uses calibrated objects or carries out calibrations itself can significantly benefit from the DCC. There are no license fees (open source).

The main advantage that can be achieved by a commercial company is that the data of the DCC is machine-readable and - when complying with the rules of good practice (GP) - even machine interpretable. This enables the introduction of accurate and trustworthy (or reliable) measurement in the Industry 4.0 environment.

2.2.4 Further advantages of the DCC

The digital transformation of the analogue calibration certificate to the DCC provides additional benefits (see Table 2).

Table 2: Further advantages of the DCC

Range of effectiveness	Impact
Industry 4.0	• Significant increase in quality assurance • Huge potential for achieving lean processes
Digital transformation of calibration	Machine-readability and machine-interpretability of the DCC's content by means of machine interaction (readability and the ability of a machine to process measurement values and formulas) lead to a significant increase in productivity in all areas of the life cycle of a calibration report.
Market potential	Companies which engage in digital transformation at an early stage can contribute their ideas as co-developers and prematurely have an advantage on the market with their knowledge.

2.3 Roadmap of the DCC

Figure 3 shows the roadmap of the DCC, with important cornerstones, connections with other projects and important events on the timeline.

Projects

Work on the DCC started at PTB in July 2017. The EMPIR [57] project "SmartCom" [58], [59] was acquired for a period of three years. In the GEMIMEGI [60] project, several representatives from industry were interviewed over a period of six months and in several workshops about topics to be researched in the future. The information thus obtained was used to draw up a research agenda which formed the basis for the application documents for the meanwhile granted GEMIMEGII [61] project. The consortium working on this project is funded by the German Federal Ministry for Economic Affairs and Climate Action (BMWK; formerly BMWi). It consists of 12 partners as well as other advisory institutions that provide further research services around the DCC over a period of 3 years [61]. In parallel, DCC-based structures for the transmission of accident data were developed over a period of three years in the ISAN project [11], [62].

Activities

The first publication on the DCC was released at the end of 2017 [1]. In 2018 and 2019, national workshops were held with partners from industry and with calibration laboratories. In September 2020, the first international DCC conference took place. More than 700 participants from more than 100 countries participated. In workshops which took place prior to the actual conference (the so-called "preworkshops"), eight working groups had been established. These worked on open issues for about one year prior to the conference. Several videos were recorded, some of which are available at the DCC website as tutorials [63]. At the beginning of 2021, topics concerning the use of the unit format known as "Digital SI" [12]" for use in digital calibration certificates were discussed at the CIPM workshop [64]. In the same year, the XXIII IMEKO World Congress [18] took place. At the beginning of 2022, the second international DCC conference followed [34]. This conference had approximately as many participants as the previous one. Then, there was an on-site event: the "Summer School". It was held in two rounds, each round for one week (the first one from 13 to 17 June 2022 and the second one from 20 to 24 June 2022). Approximately 40 persons took part in each round. In the autumn of 2022, the IMEKO TC6 M4DConf [39] was held. Shortly afterwards, there was the Digital NIST Workshop [40], [65] and, at the beginning of 2023, the third international DCC conference [42] (see section 2.4).

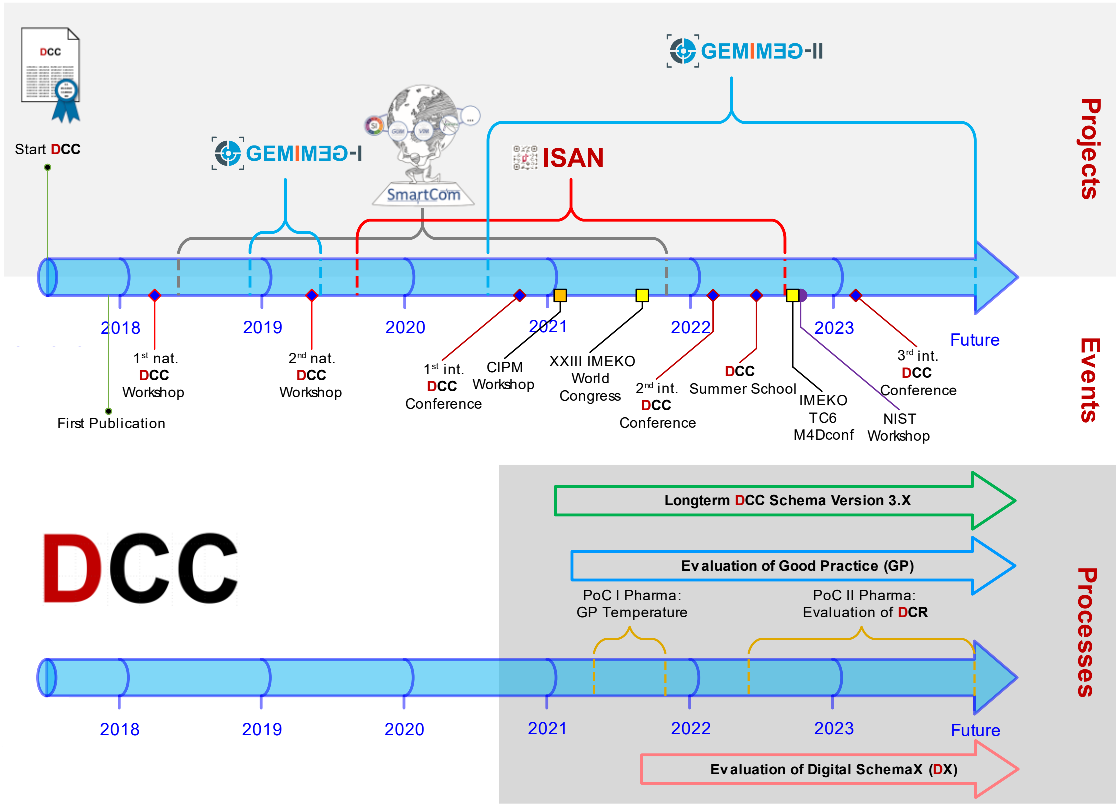

Figure 3: Roadmap of the DCC

Processes

Starting in 2021, the first proof of concept (PoC) was carried out for the DCC in an industrial application with representatives from the pharmaceutical industry and an accredited calibration laboratory. This laid the foundation for the GP (Good-PracticeDCC-, see section 3.2.2) for temperature calibration. Shortly before that, version 3.0.0 of the DCC-XML-Schema had been published. This version is designed in such a way that all versions of series 3.X.Y are long term available, which was a decision that was of great importance to the partners from industry. Furthermore, the necessity for introducing a DCR (digital calibration request) and a DCA (digital calibration answer) was identified. A GP-DCC for temperature calibration has been published on the DCC website [66]. Later on, further GPs (for the calibration of ambient pressure and for air humidity sensors) were published [66]. Moreover, an initial report was issued by experts of the German Calibration Service (DKD) on creating a DCC for weights [67]. In the middle of 2022, the second proof of concept (PoC II) was carried out with the aim of supporting the idea of the DCR and the DCA more strongly. The development of schema versions - summed up under the acronym “DX” - had already been started during the processing stage of PoC I.

2.4 Results from the third international DCC conference

For the first and the second international DCC conference, quite a large number of participants from all over the world had registered. At the third conference, the number even rose to 1146 participants from 93 countries.

To the third international DCC conference [42], all interested parties working on the topic of “Digitization and Digitalization & Digital Transformation” in the field of calibrations were invited to present their versions of the digital calibration certificate. at the conference. Furthermore, they were invited to report on their own developments in the field of digital certificates. For that reason, it can be assumed that an approximately representative number of involved persons from all over the world had the opportunity to present their work and their solutions with regard to this topic at this conference.

Altogether, 57 applications for presentations were submitted. The conference was coordinated by an international programme committee. This committee decided to permit 56 presentations to be held at the conference. After the conference (during which all the approved presentations were actually held), these presentations were classified (Table 3).

Table 3: Classification of the presentations

Total number of presentations held: Out of which:	56
• Not focused on DCC topics:	10
• PTB presentations incl. DCC:	15
Remaining:	31
Out of which: • PDF/A3 only:	1
• XML-Schema-based XML	26
• XML-Schema-based XML in PDF/A3	4

It showed that the vast majority of presentations on the DCC dealt with the XML-only variant of the PTB-coordinated DCC. Only one presentation dealt with the sole use of PDF/A3. Some presentations reported on the “PDF/A3 with validated DCC XML” variant, based on the PTB-coordinated DCC.

3 Digitization versus Digitalization & Digital Transformation

3.1 Preliminary remarks

It is indisputable that every year, several millions of calibrations are carried out worldwide. The aim of this publication is to make clear how important the DCC is for all those who deal with calibrations - and especially with the results of these. An important aspect is to avoid media discontinuity. This prevents faults that might occur during the (currently common) practice of transferring an analogue calibration certificate (paper!) into a machine-readable or - even machine-interpretable - digital document. However, it is questionable whether a calibration certificate in the form of a PDF document can fully avoid this media disruption. One question that should be investigated in particular is: How do the different procedures turn out with regard to “Digitalization & Digital Transformation”?

Free choice of the cryptographic methods

What customers expect from a calibration is the legally binding certainty that the data will be consistent. This means: The data that has been created by the issuing calibration laboratory and which is, later on, transmitted via an arbitrary information channel must correspond to the data that has originally been created by the calibration laboratory. This is a very important issue. Within the scope of the GEMIMEGII project [61], a further issue is being investigated: that of a legally secure measurement and calibration chain [68] for complex sensor networks (international law).

The PDF/A3 format, however, does not comply with the general security requirements of free choice of cryptographic methods because a fixed format is prescribed. (see section 0 Contra 9 (PDF/A3 only)).

In the sector for which the calibrations are mainly carried out, the efficiency of the processes is important. And such efficiency is especially important in the context of Industry 4.0.

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Unambiguity of the data structure

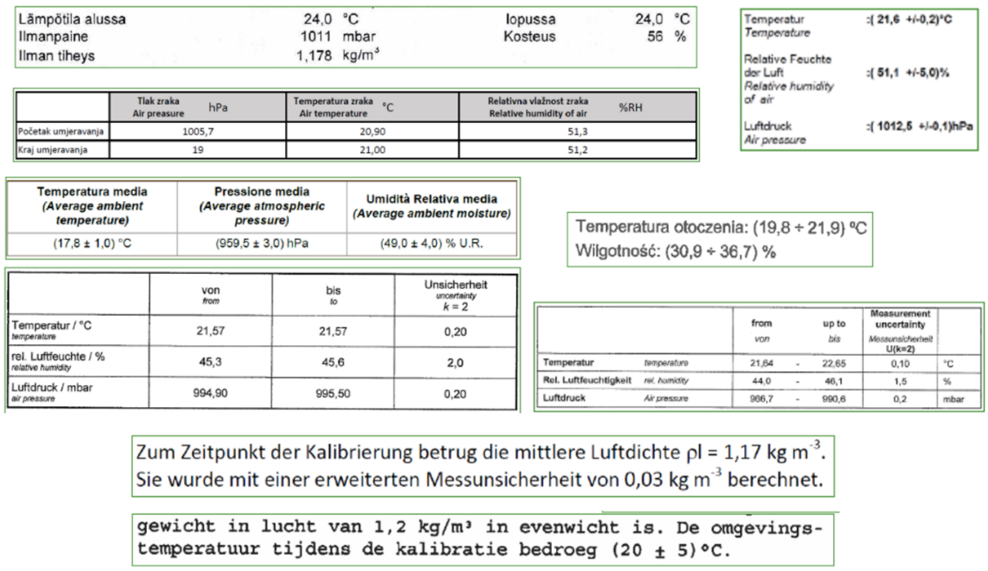
Another important issue is that the data structure must be unambiguous. This unambiguity is defined worldwide by the DCC Schema. In addition, faultless data, and the potentially high increase in quality play an important role.

When we compare the methods with each other, the following can be observed: So far, a text processing template has mostly been used, which has been filled in, printed, then scanned and then converted into a PDF document using OCR (optical character recognition [69]) software. Then some went over to converting the text processing template directly into PDF, or a PDF template was used. Now, also LaTeX templates are used.

3.2 Humans and machine; good practice (GP), fault reduction

3.2.1 The ability of humans

Humans are able to process complex connections, especially when they have specialized in a certain task. A person with the respective prior knowledge of metrology is able to analyse and evaluate complex connections in the field of metrology. Figure 4 shows a compilation of different calibration certificates which are all about ambient conditions of the same issue (mass piece). These certificates can all be evaluated by specialized humans.



Lämpötila alussa	24,0 °C		lopussa	24,0 °C
Ilmanpaine	1011 mbar		Kosteus	56 %
Ilman tiheys	1,178 kg/m³			

	Temperatur Temperature	:(21,6 +/-0,2)°C
	Relative Feuchte der Luft Relative humidity of air	:(51,1 +/-5,0)%
	Luftdruck Air pressure	:(1012,5 +/-0,1)hPa

	Tlak zraka Air preasure hPa	Temperatura zraka Air temperature °C	Relativna vlažnost zraka Relative humidity of air %RH
Početak umjeravanja	1005,7	20,90	51,3
Kraj umjeravanja	19	21,00	51,2

Temperatura media (Average ambient temperature)	Pressione media (Average atmospheric pressure)	Umidità Relativa media (Average ambient moisture)
(17,8 ± 1,0) °C	(959,5 ± 3,0) hPa	(49,0 ± 4,0) % U.R.

Temperatura otoczenia: (19,8 ÷ 21,9) °C
Wilgotność: (30,9 ÷ 36,7) %

	von from	bis to	Unsicherheit uncertainty k = 2
Temperatur / °C temperature	21,57	21,57	0,20
rel. Luftfeuchte / % relative humidity	45,3	45,6	2,0
Luftdruck / mbar air pressure	994,90	995,50	0,20

		from von		up to bis	Measurement uncertainty Messunsicherheit U(k=2)	
Temperatur	temperature	21,64	-	22,65	0,10	°C
Rel. Luftfeuchtigkeit	rel. humidity	44,0	-	46,1	1,5	%
Luftdruck	Air pressure	986,7	-	990,6	0,2	mbar

Zum Zeitpunkt der Kalibrierung betrug die mittlere Luftdichte ρl = 1,17 kg m^{-3}.
Sie wurde mit einer erweiterten Messunsicherheit von 0,03 kg m^{-3} berechnet.

gewicht in lucht van 1,2 kg/m³ in evenwicht is. De omgevings-
temperatuur tijdens de kalibratie bedroeg (20 ± 5)°C.

Figure 4: Representation of ambient conditions from different calibration certificates of the same issue (mass piece) [70]

3.2.2 Good practice (GP)

Preliminary remarks

Calibrations are relevant for a very wide range of scientific and engineering processes. Depending on the content to be calibrated, they can, however, be very different. For example, a calibration certificate on mass determination differs significantly from a calibration certificate on force, although these physical quantities are connected with each other. For different sectors, different rules, norms and standards exist which, in part, lay down precisely what the calibration certificates issued in a specific field of work have to include. Due to the fact that calibration certificates often strongly deviate from each other, it makes sense to agree on a uniform format. This agreement can, however, only be achieved in calibration-specific sectors where the respective communities can work together on a harmonized format.

Analogue world

The GP approach is to be seen independently of the Digital Transformation, as a uniform presentation of calibration results in calibration-specific areas creates a comparability that is also easier for humans. For Figure 4, this would mean that the results of the ambient conditions would all be indicated in one and the same form.

Digital transformation

The GP approach is - of course - very important for the digital transformation. Apart from the elements which have already been unambiguously defined, and apart from the centrally managed attributes, all community-specific attributes have also been unambiguously defined. Furthermore, the design of the XML itself is clearly regulated within the community. This will be explained in section 0 by means of an example.

3.2.3 What do the machines need?

Machines need data that is unambiguous and interpretable worldwide. Otherwise, it would not be possible for them to identify and process the data in a legally secure way. The data shown in Figure 4 is useless to a machine.

Calibration certificates which are rich in content

When a calibration laboratory has produced large amounts of data, it might be the wish of the customer that all of this data is included in the DCC.

A limitation by the number of paper pages per document is then not expedient. Similarly, it is not very useful to hand over a large number of pages in PDF (or even on paper) to the customer.

Due to the machine readability and machine interpretability of the DCC, it is easy for algorithms to extract the required data without faults even from comprehensive DCCs. In principle, this extraction process is also applicable in the case of paper documents. This, however, is possible with high manual effort only and bears the risk of faulty results. In the example where the calibration results are also available as a PDF file, the tables will have the same column headers on each page. These headers are redundant information and impede an automated search.

Avoidance of faults

An important advantage of digital transformation is that faults are avoided. This is due to the fact that an automatic check is carried out by means of the DCC Schema and an analysis can be performed using Schematron [71].

What is of great importance here is that the respective rules, norms and standards are observed. More than half of all calibrations are carried out by non-accredited calibration laboratories, see Figure 1. The DCC is also designed for these calibrations, even if not all rules of ISO/IEC 17025 [50] are necessarily applied there. In accredited calibration laboratories and the NMIs/DIs, the requirements of ISO/IEC 17025 shall be fulfilled. It is very important for these institutions to comply with the rules, which are checked by internal and external audits. GP-DCCs contribute significantly to passing these audits without complaints because of the unified structure as well as the error prevention supported by software tools. In a DCC, the results of such audits are stated in such a way that they can be understood by the entire expert community worldwide. The reason for this is that the DCCs are all very similar to each other. At the third international DCC conference [42], a whole series of presentations was held on this topic, summarized under the category of “DCC and Machines”. Another category was the group of topics called “DCC and Industry”.

And what about human readability?

There are several possibilities to create a human-readable equivalent from an XML file. For example, the XML Notepad software by Microsoft [72] is available to everyone as it is public domain. It can be used to view the entire content of the XML file. Furthermore, there are also commercial software products such as XMLSpy by Altova [73] or Oxygen [74].

For auditors, it is of great advantage to find a uniform version as their work becomes more objective in this way. A great number of software tools can be used for the audit. It is, of course, possible to make a conventional human-readable version available to the auditor. As far as this topic is concerned, please refer to the various presentations of this conference [42], especially in the categories of "Human Readable DCC" and "DCC Tools", as well as to the presentations which were held with regard to commercial products that are available for the DCC.

3.3 The utility model

The issues mentioned so far refer to the topic of "digitization", but not to the topic of "digitalization & digital transformation". There is an important difference between them which will be explained in the following by means of the *utility model*.

This model was developed by a working group [75] of the International Organization for Standardization (ISO [76]). In Table 4 below, the different levels of the model are described.

Table 4: The different levels of digitization and digitalization

Level	Remark
Level 0	Hard copy (paper)
Level 1	The document is available in digital form, for example as a PDF file
Level 2	A machine-readable document, for example an XML file without structural information, such as a publicly accessible and described schema.
Level 3	At this level, we have obtained machine-readable and machine-executable data. The reason why the data can be executed by machines is because the content is exactly described by means of meta data. This is the case when the XML file has been validated against the structure of a known and defined schema. This is exactly what can be done with the DCC: a validation against the DCC Schema. There is a clear definition available of what is stored in the elements of the DCC.
Level 4	The aim at this level is machine-interpretability, which can be achieved with Good Practice (GP) DCCs. At this level, each DCC which is based on Good Practice from a field of metrology is described unambiguously. A machine can be programmed on the basis of GP DCCs in such a way that it is able to interpret GP DCCs. The machine can then also interpret new DCCs which were created by using GP DCCs as a template.
Level 5	At this level, the stage is achieved where the content of a DCC can be controlled by a machine (i.e., machines can interpret the content of DCCs completely on their own). The content of a norm or standard can be adjusted and adopted automatically by machines due to automated decision processes. The digital norms and standards are based on an Artificial Intelligence system that has cognitive abilities. Digital norms and standards are able to continuously adjust themselves to the current state of knowledge of the technical and regulative framework conditions.

By means of "digitization", only level 1 can be achieved, however not level 2, where "digitalization" and "machine-readability" are achieved for the first time. The aim is to achieve at least level 3, or even better, level 4. Figure 5 illustrates this connection. The production processes of today have to be digitalized and digitally transformed to increase productivity and, at the same time, improve the quality of products and services.

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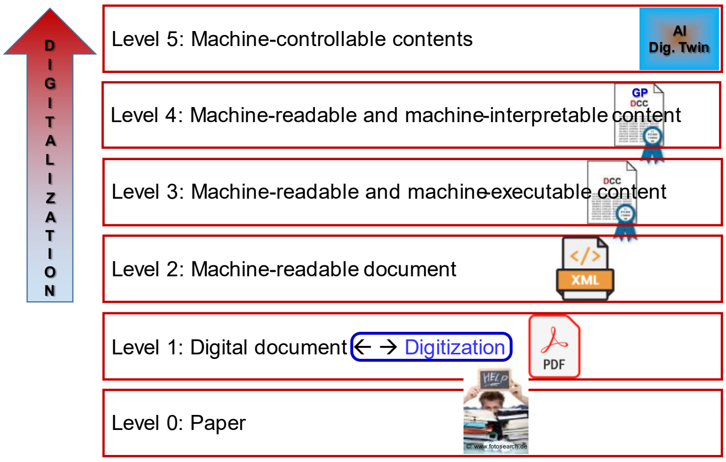

Figure 5: Explanation of the difference between "digitization" and "digitalization" by means of the utility model (based on [75])

3.4 Level achieved by the DCC in the utility model

Preliminary remarks

The DCC developed by PTB in cooperation with the international community of NMIs, calibration laboratories and industrial partners is analysed in more detail below and classified using the utility model. The requirements for the different levels of the utility model are built upon each other. Thus, a digital representation is a prerequisite for level 1. Digital representation is also a necessary prerequisite for levels 2 - 5. For level 2, a structured data format is also necessary, but software processing is only possible with great manual effort. This is the case, for example, if an XML document is used which has an - only locally known - "Document Type Definition (DTD [77])" or an XML Schema.

Level 3

The DCC that is being analysed in detail below is - in its generally useable form (i.e., without applying any further rules, norms and standards) - to be assigned to level 3. The minimum requirements for this level are:

1. The document is available in digital form (from level 1).
2. A structured document format is available (from level 2).
3. The content is completely (semantically) deciphered.
4. Semantic search and selective access at the content level are possible.
5. The information contained in one document is transmitted to several other documents one after the other, but only for a specific purpose.

Items 1 and 2 above are complied with by the fact alone that the DCC that is being analysed here is a format that is based on XML.

With the DCC, it is, however, still (additionally) possible to indicate all the information that is relevant for creating calibration reports in accordance with chapter 7.8 of ISO/IEC 17025:2018 [50]. This was also notified in a joint press declaration of the *Deutsche Akkreditierungsstelle* (DAkkS) (German accreditation body) and PTB [78] and means that the requirements of item 3 above are fulfilled as well because the XML schema used is published [79].

Item 4 refers to the actual core of the publication of the utility model: the norms and standards. However, the DCC is not a norm or standard. It is therefore debatable whether this item can be applied to the DCC. But as all element names in the DCC are derived from names of the standardization environment of the DCC, the preconditions for a semantic search are given. For example, if you find a specific term in ISO/IEC 17025 and you find a similar element name in the DCC, you can assume that this is the search result. Another approach is the use of attributes with the name “refType”, which are embedded in a clearly defined context. The selective access at the content level is possible in that case, for example, with mechanisms from the XPATH environment [80].

Item 5 is also regulated via the selective access. The requests are identical for all DCCs and thus provide comparable results. For this reason, it is possible to evaluate key-comparisons with a high efficiency and high quality.

Level 4

Compared to level 3, level 4 includes in addition:

6. Information models that describe and explain the content and the relations between pieces of information
7. Self-learning analysis as well as automatic validation and optimization
8. Value added services are possible, such as e. g.:
    - conformity assessment
    - question answering
    - predictive content supply
9. An uninterrupted digital value chain is possible

For all of these items it must be taken into account that the publication on the utility model [81] is geared to the machine-interpretability of norms and standards and that this model is therefore not unambiguously applicable to DCCs. The properties which are mentioned in the text below presume that for a specific category of calibrations, a uniform format is used for the DCC. This is summarized under the term “Good Practice (GP see section 3.2)”. The result is, in this case, a DCC design which always has one and the same appearance for a specific class of measurands. Examples of GP-DCCs are:

- temperature
- air humidity
- ambient pressure
- Soon, the following will be available:
    - mass and weight
    - force
    - torque
    - non-automatic weighing instruments
    - gauge blocks

Item 6 is already covered by the reference to the attributes named “refType” mentioned under item 4. Furthermore, there are clearly defined and unambiguous identifiers (e.g. in the element dcc:equipmentClass) to classify and identify specific devices unambiguously. For this, special systematics are already available that could be used here. It is, for example, possible in the case of weights to refer to OIML R 111-1 [82].

Item 7 refers to the possibility of inserting devices into the overall production process (e.g., via the asset administration shell of the Industry 4.0 environment) which then enables a self-learning analysis as well as automatic validation and optimization.

The value-added services listed under item 8 have, in part, already been implemented in item 5. These processes can also be immediately connected to Industry-4.0 components, making, for instance, the field of total quality management much more efficient and thus saving resources.

Item 9 is therefore covered automatically as all the data of the calibration object is available and useable and can, for example, be integrated into the “Digital Product Pass (DPP)”.

3.5 *Digitization* versus *Digitalization & Digital Transformation* using, as an example, a comparison of calibration certificates for weights

Explanation of our example

In the following, we will show the differences between "digitization" and "digitalization & digital transformation" by means of an example. In Figure 4 (section 3.2.1), the results of different ambient conditions for the mass calibration of weights and weight sets are compiled. By means of this compilation, the results of different calibration laboratories can be compared. The ambient conditions are always of the same type, but the different laboratories use different ways to represent them.

Representation at level 0 or at level 1

All the calibration laboratories have issued their results as hard copies or as PDF files. This means that the calibration certificates are available at level 0 or level 1, respectively of the utility model. Even at level 1, it will only be possible for a human expert to assess these different representations of ambient conditions as the data has not been processed to be used by a machine. In this context, it is necessary to take a closer look at the details. Currently (in September 2023), it must be stated that machines are still just machines. It is true that there is, for example, AI [83]-based software [84] that might be able to pass the Turing test [85]. But these systems need high computing power and a large amount of data to be trained with, which means that an extremely high input of energy is necessary. In contrast to this, it is most important for the end users to be able to use the data of the DCC as efficiently as possible for their production and saving resources at the same time. To complicate matters further, the sensors used in this field usually only have very low computing power or even just an analogue-to-digital converter [86].

Representation at level 2

Let us assume that each calibration laboratory has stored its calibration certificates in an XML-based format. However, each calibration laboratory uses its "own" XML, which deviates from the other XML structures that are in use. Then the XML files are readable by machines. However, it is not possible to assign the contents of the XML files and then execute or even interpret them. The reason is that the contents of the elements cannot be "mapped", i.e. assigned to each other. Figure 4 shows extracts from the calibration certificates of nine calibration laboratories. In these certificates, the ambient conditions are stated in very different ways and the ambient temperature is indicated in seven different languages. Extracting the ambient temperature is not possible. The same applies if laboratories use an unpublished and undocumented XML Schema or a Document Type Definition (DTD [77]).

From level 2 of the utility model onwards, it would already be possible for each calibration laboratory to generate its own individual human-readable version from the XML file. But it would not be possible to exchange the files with each other.

Representation at level 3

At level 3, all calibration laboratories use a clearly defined, uniform XML Schema. This is the DCC Schema which was coordinated by PTB. Now it is possible to exchange the data with each other. Due to the existing definition of the elements and attributes of the XML Schema that belongs to the DCC, level 3 of the utility model has now been reached. A machine is able to process and execute the data, but not to interpret it.

The contents of the elements can be extracted by means of the description. In the example shown in Figure 4, it becomes clear due to the structure of the XML file that it is about ambient conditions. In the same way, the information about the calibration object, the calibration laboratory, etc. is unambiguous in accordance with section 7.8.2 of ISO/IEC 17025. Due to a generally valid set of identifiers of attributes, it is possible to extract the different ambient conditions. In this way, the linguistic variety (e.g. for indicating ambient conditions) is eliminated. The elements which contain the information about temperature can be clearly extracted.

At this point, however, the calibration certificates are not yet machine-interpretable. This will be discussed in section 0.

Representation at level 4

As explained in section 3.2.2, using GP is an important factor for digital transformation. Applied to our example, this means that apart from the unambiguously defined elements (see 0 above) and the centrally managed attributes, all community-specific attributes have also been unambiguously defined. Furthermore, the design of the XML itself is clearly regulated within this community.

Let us assume that all the DCCs of our example have been created according to the GP rules of the respective community. What is striking in the first place is that not all calibration laboratories have kept to these rules. For example, some calibration certificates do not show the ambient conditions for ambient pressure, or the units have not been harmonized. These deficits can already be avoided in the calibration laboratory by means of software-based automatic monitoring. The respective method for this (analysis using Schematron) has already been mentioned in section 0 above. Another method is to submit the exact calibration order via a digital calibration request (DCR). This method, however, will not be addressed in this publication.

After all the calibration laboratories have now generated and delivered a valid GP following the internal audits, the DCCs can now be further processed in a machine-interpretable way. Based on the GPs, the machine can then generate various evaluations. It is, for example, possible to generate a dataset for a key comparison at any time without any transmission faults occurring.

4 PDF versus XML

Preliminary remarks

As part of the DCC projects, freely available and simple software tools are being developed which will raise the usability for XML to a high level of convenience. These tools were presented at the DCC conference [42]. Further tools from the community are under development. In the foreseeable future, these tools will be publicly available.

It needs to be stressed that PDF files are only readable if the corresponding software (the so-called “viewer”) is available on the respective program system. When both filetypes are opened next to each other in the editor, it quickly becomes clear which file is more easily readable for machines. Thus, all users need a tool to represent documents in a way that can be read by humans.

Beginners and experts who want to have full control should use text editors such as Notepad++ [87], Editor [88], Ultraedit [89] or XMLPad [90] or comfortable programming environments such as Visual Studio Code [91], XML Notepad [72], Oxygen [74] or Altova XMLSpy [73]. For some of these, charges may have to be paid.

When a text processing file is exported into a PDF format, the same happens as when a DCC (XML) file is exported into a PDF document. What needs to be clarified, however, is whether the attachment of digital data of the PDF solution actually meets the requirements of the SI Digital Framework [92]. The question remains whether the security of the entire digital data that is available in the document can be ensured and whether the FAIR principles [56] are complied with, etc. If this is the case, then the whole process is not only about digitizing data but creates the basis for the digital transformation of data.

4.1 Comparison between XML and PDF/A3

Preliminary remarks

The following comparison is not about data or formats, but about the structure or philosophies of XML and PDF/A3. For that reason, the two fundamentally different approaches are to be compared as a first step.

Advantages

Table 5 contrasts the advantages of XML with those of PDF/A3. Below this table, the individual numbers are further explained.

Table 5: Advantages of XML and PDF/A3

Pro XML	Number	Pro PDF/A3
XML is internationally standardized and is very well suited for long-term storage.	Pro 1	PDF/A3 is internationally standardized and is very well suited for long-term storage.
XML can serve as a container for files.	Pro 2	PDF/A3 can serve as a container for files.
If the calibration laboratory and the end user work with an XML file right from the start (which will not be noticeable due to the tools), an additional migration step (from PDF/A3 to XML) will be avoided later on.	Pro 3	Everyone knows PDF files and they are easy to understand. They are often used by authorities and administrative offices.
XML has been tried and tested, has been used on a broad scale for more than 25 years and is already human-readable in this form for trained users.	Pro 4	Not much time needed to familiarize oneself with it, i.e. it has been used for a long time and is therefore well known.
Human-readable versions are supported in several formats.	Pro 5	
It is possible to use modern viewers such as HTML.	Pro 6	
Free choice of signature and encryption algorithms	Pro 7	
The stakeholders may choose the certification bodies.	Pro 8	
Permits the pure exchange of data without the fourth area of the DCC [1].	Pro 9	
The DCC is complete.	Pro 10	
Conversion into other formats is ensured without loss of information.	Pro 11	
Utility model: Level 3-4	Pro 12	

Pro 1 (XML and PDF/A3)

XML:

XML was first published in February 1998 and has thus been standardized for more than 25 years [93]. The data can be opened with a simple text editor. The content indicated in the elements and attributes is readable according to international standards.

PDF/A3:

Please see the respective standard [94].

Pro 2 (XML and PDF/A3)

Preliminary remarks on both file formats

Both file formats can carry any files in any data formats in a data container. However, it is not sufficient to only embed the original files (e. g. text processing or spreadsheet files, etc.) in the document or to attach them to the document for archiving purposes, as it cannot be guaranteed that it will still be possible to open these attachments in ten years. This does not apply to XML files, as these are text files. Further details were already drawn up in 2013 [68].

XML:

For more than 25 years, XML has been able to store arbitrary data as a character string via lossless coding/decoding (such as the Base64 method) [95].

PDF/A3:

The aim of the PDF/A (archive) format is the long-term availability of the included information. All file types (original files) can be included in a file in PDF/A3 format via the “attachment of digital data”.

PDF/A3, too, permits the embedding of arbitrary file types, but requires more than what is usually required in ISO 32000-1 [96] or ISO 19005 [94] for “normal” PDF 1.7 files. Files that meet these requirements are called “associated” files. The generating program has to create an explicit association between each embedded file and the PDF file which contains this embedded file (or an association with the object or structure that is contained in that PDF file). In the XML file, this association is ensured by means of its transparent and machine-readable structure.

Pro 3 (XML and PDF/A3)

XML:

At the third international DCC conference [41], it was seen that the vast majority of presentations dealt with the XML-only variant of the DCC. Only one presentation dealt with the sole use of PDF/A3-based documents. Some presentations reported on the “PDF/A3 with validated DCC XML” variant. Further details on this can be found in section 2.4. If international uniformity can be achieved, then the calibration laboratories and the end customers that have agreed upon an integral XML-based solution right from the start will not need another migration step.

PDF/A3:

For those who are purely consumers, files in PDF/A3 format are well established and immediately human-readable when using PDF readers that are available free of cost. In this way, the 1:1 “digitization“ of the classical paper formats such as DIN A4 [97] or US Letter [98] is achieved.

Pro 4 (XML and PDF/A3)

XML:

XML is very common in the field of IT and is implemented in many applications. The data can be opened and viewed by means of a simple editor. Users only need a short familiarization time to be able to comprehend the content. This is especially facilitated by the fact that the description of the elements and attributes is available. For further information, refer to [46].

PDF/A3:

Those who are purely consumers are surely familiar with PDF documents as such documents are part of everyday life, for example in the form of bank statements or official documents.

Pro 5 (XML only)

The human-readable part of the DCC is created according to the customer’s specifications. This is possible because ISO/IEC 17025 Section 7.8 only regulates what is expected in the result report. This is represented by the two inner areas of the DCC. The customer therefore does not need the human-readable part of the DCC.

For that reason, the customers can choose between different formats, for example PDF, HTML5, DOCX, etc. All output formats that the calibration laboratories can generate and that are human-readable are possible. The calibration laboratories can export all formats into the fourth area of the DCC in a lossless and unambiguous way.

Pro 6 (XML only)

This opens up much better viewing possibilities, especially for extensive calibration results. HTML5 no longer has any page breaks. Further active HTML5 elements can be integrated (for example, rearranging tables).

Also, there are, in principle, no limitations to the scope of an output. Thus, a human-readable calibration result report of several hundred pages in DIN-A4 format would be possible.

Pro 7 (XML only)

The customer and the calibration laboratory can choose and apply any method whatsoever to ensure the integrity and authenticity of the calibration data. Both contracting partners are also free to choose the methods that should be applied because they are based on mutual trust between the two partners.

This aspect is especially important in areas in which the regulations of a state or of a company, for example, only allow specific methods that cannot be represented by means of the PDF/A3 format.

Pro 8 (XML only)

Customers may freely decide which trust service provider they want to choose. Here, the same applies as in section Pro 7: that in some areas, a trust service provider is prescribed who is not implemented in PDF/A3.

Pro 9 (XML only)

The following fault is eliminated: The leading data from the two inner areas of the DCC does not correspond to the human-readable content in the outer area of the DCC. According to ISO/IEC 17025, the two inner areas of the DCC are sufficient as the result report is already stored here.

Pro 10 (XML only)

Whether a DCC is complete can be checked by means of schema validation and other tools (e.g. Schematron).

Pro 11 (XML only)

Conversion of the file into other formats is possible without any loss of information as the structure and content of the elements and attributes are made accessible. Some of the converters are currently being worked on within the scope of the GEMIMEG-II project [61].

Pro 12 (XML only)

With regard to this point, refer to section 3.4.

Disadvantages

Table 6 contrasts the disadvantages of XML with PDF/A3. Below this table, the individual numbers are further explained.

Table 6: Disadvantages of XML and PDF/A3

Contra XML	Number	Contra PDF/A3
The enclosed human-readable version has to be extracted and converted from the XML beforehand before it can be viewed.	Contra 1	A viewer is always required (as a matter of principle, XML does not need the viewer).
It seems more complicated than the signature and encryption in the PDF document.	Contra 2	If the end user works with an XML file right from the start (which will not be noticeable due to the tools), an additional migration step (from PDF/A3 to XML) can be avoided later on.
Easily understandable software for validating the DCC via XML signature in XML documents still needs to be developed.	Contra 3	A human-readable document is always required.
	Contra 4	Using the DCC Schema can be completely circumvented because all data is transferred without verification.
	Contra 5	It is not clear whether the DCC is complete.
	Contra 6	The XML file must be extracted first.
	Contra 7	Utility model level 1
	Contra 9	The Adobe company has the monopoly position in signature and encryption algorithms supported by the PDF format as well as in selecting the certification bodies.
	Contra 10	As Adobe PDF is proprietary, security gaps may remain undetected for a long time.

Contra 1 (XML and PDF/A3)

XML:

Within the scope of the GEMIMEG-II project, a solution has been developed that is freely available [47]. The authors have also been shown developments from industry where internal solutions have been developed. At the third international DCC conference, several manufacturers presented their solutions.

PDF/A3:

PDF/A3 is not readable without a viewer, see section 0.

Contra 2 (XML and PDF/A3)

XML:

The user interface for the signature and encryption that most users have is not very user-friendly yet. The GEMIMEG-II project is currently working on this issue.

PDF/A3:

At the third international DCC conference, it was seen that only a minority of presentations dealt with the PDF/A3 variant of the DCC. Further details on this can be found in section 2.4. If international uniformity is achieved, the calibration laboratories and the end customers that had initially favoured the PDF/A3 solution will need another migration step.

Contra 3 (XML and PDF/A3)

XML:

The user interface for validating the signature and encryption that most users have is not very user-friendly yet. The GEMIMEG-II project is currently working on this issue.

PDF/A3:

Here, a human-readable document would have to be declared to be a mandatory field as a PDF file is, by definition, intended for displaying human-readable content.

Contra 4 (PDF/A3 only)

The disadvantages, especially the risk that the validation might be circumvented (Contra 4), are very critical for DCCs that are issued by accredited bodies.

Contra 5 (PDF/A3 only)

The disadvantages, especially the risk that the check for completeness might be circumvented (Contra 5), are very critical for DCCs that are issued by accredited bodies.

Contra 6 (PDF/A3 only)

This means an additional step in the process chain.

Contra 7 (PDF/A3 only)

For this point, refer to section 3.4.

Contra 9 (PDF/A3 only)

The standardization of PDF/A3 did not take place with the necessary openness when selecting the signature and the encryption algorithms. Neither was it possible to select certification bodies. This restricts the use of PDF/A3, which can lead to the fact that it does not fully work in certain environments (e.g. in countries or organizations) from the cryptographic point of view.

Contra 10 (PDF/A3 only)

Adobe PDF is proprietary and therefore bears the risk of undetected security gaps. In 2019, a security gap led to the fact that forged signatures were not detected [99].

4.2 Signatures

Signatures are integrated into the XML files via an additional schema. This signature schema is a signature schema that is hardened against an XXE attack [100] on the basis of the respective W3C schema [100]. The XXE attack is avoided by not using the "Document Type Definition (DTD [77])". The DTD is not necessary because CDATA elements [101] are not used in the DCC due to a decision made at the first international DCC conference. This decision was also based on security reasons, as CDATA elements are a gateway for malware.

The DCC Schema that is coordinated worldwide by PTB is available to the general public (open source) and can contain all kinds of signature methods. PDF/A3, however, is specified and regulates the signature methods.

In the case of PDF/A3, embedded content can be co-signed. However, it is questionable whether this makes sense at this point. Especially in the field of the automatization of production processes, an integrity check can be carried out automatically. If the integrity check is intended to be carried out via a PDF/A3 document, then the entire human-readable content has to be provided up to the machine that is to process the XML document. This is because the entire content as such must be available to check the signature.

It could be argued at this point that an XML signature could be applied to an XML document nevertheless to have a separate signature available, independent of the human readable version, as part of the PDF document. However, this would make PDF/A3 obsolete as a de-facto standard for signatures and turn it into a mere container format.

4.3 FAIR

Another important aspect that should be addressed is FAIR data. The basic principles of FAIR data are: Findable, Accessible, Interoperable, Reusable [56].

The question here is whether XML DCCs and PDF files with embedded XML files meet the FAIR principles. An analysis has shown that the XML DCCs meet all four criteria. However, this does not apply to PDF documents because they are not interoperable in this form, mainly due to the fact that a clear definition of meta data is missing. Each calibration laboratory defines meta data in a different way. In contrast to this, the DCC Schema offers a clear definition of the meta data.

4.4 PDF/A3 with validated DCC-XML

Preliminary remarks

What happens when a PDF/A3 contains a validated DCC-XML file according to the PTB-coordinated DCC Schema? At the third international DCC conference [42], some presentations dealt with this variant (see section 2.4).

The issuance of a report with regard to the three inner areas of the DCC according to the PTB-coordinated DCC is identical. The two variants differ from each other in two ways:

- the storage methods for the three inner areas of the DCC
- the handling of the human-readable version

These differences will be addressed in the following.

Storage methods for the three inner areas of the DCC

In the case of the PTB-coordinated DCC, the three inner areas of the DCC and the human readable part (fourth area of the DCC) are stored in one single XML file so that the content of the entire DCC can be processed with one toolbox.

In the case of the PDF/A3 variant, the XML file with the three inner areas of the DCC must first be extracted from the PDF file, which requires an additional tool. This will also be highlighted in the section 0.

Handling the human-readable version

For this purpose, the XML file must first of all be extracted from the PDF file. This additional step has to be carried out by the end user in the industrial environment. An auditor can only assess the content and view the entire DCC afterwards. In concrete terms, this involves several disadvantages:

- Being fixated on only one PDF document.
- Not being able to change to other formats.
- Displaying large tables without pagination is not possible.
- An additional step is required to extract the XML file from the PDF file.

5 Summary and outlook

At the beginning, we presented the DCC that is coordinated worldwide by PTB. An overview of the development of the DCC and its roadmap was given. Based on the discussion with regard to the third international DCC conference, the topic “*Digitization* versus *Digitalization & Digital Transformation*” was then addressed. The fundamental difference between the two terms was made clear. In doing so, the utility model was explained by means of an example. These analyses were then included in a comparison between the approach of the PDF/A3-based DCC, on the one hand, and the XML-based DCC Schema which was coordinated worldwide by PTB on the other hand.

This publication contributes to achieving the worldwide uniformity of the machine-readability and machine-interpretability of calibration results in the form of Digital Calibration Certificates (DCCs). This uniform course of action offers the opportunity to optimize global trade. Each trading nation in the world is capable - within the scope of its overall economy - of optimizing its trade relations and therefore has all the possibilities of saving any natural resources. The partners from industry expect, from their respective national metrology institutes, a uniform course of action which extends across the entire field of metrology. One of the first steps here could be achieving the use of uniform language elements in the worldwide coordinated DCCs.

6 Miscellaneous

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