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PROMISING BENEFITS OF AN SELF-UPDATING (U)DCC APPLICATION EXAMPLE: THE QUANTUM-BASED PASCAL

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Abstract – The DCC enables an updatable and thus improvable uncertainty budget. A direct benefit of the updatable DCC (UDCC) for the device under test (DUT) and thus for the end users would be the transfer of improvements with respect to the uncertainties of the primary standards. An illustrative application example is the new realization of the Pascal via quantum-based methods, such as primary standards using Fabry-Perot (FP) refractometry. This novel realization is based on traceability by means of frequency measurements and it is expected that the uncertainties of the relevant fundamental quantities, such as the polarizability and virial coefficients of the gases used, will improve noticeably on a regular basis over the next years. The resulting reduction in the uncertainties of all corresponding primary standards can be passed on directly to the end user due to the advantages of the machine-readable (and potentially machine-interpretable) digital calibration certificate which makes it well updatable.

Keywords: Updatable DCC, UDCC, machine-interpretable, improvable uncertainties, redefined SI, quantum-based Pascal

Abbreviations:

CDG	capacitance-diaphragm gauge
CMC	Calibration and Measurement Capabilities
DCC	digital calibration certificates
DUT	device under test
FP	Fabry-Perot
FPC	FP-cavity
GAMOR	gas modulation refractometry
GUM	Guide to the Expression of Uncertainty in Measurement
QP	QuantumPascal project (EMPIR 18SIB04)
SOP	stationary optical pressure standard
TOP	transportable optical pressure standard
UDCC	updatable DCC

1. INTRODUCTION

In this article, the advantages of an updatable digital calibration certificate (UDCC) are shown by means of exemplary application examples considering two devices under test (DUT) in a fictional but not unrealistic scenario. DUT1 is a conventional capacitance diaphragm gauge (CDG) designed for the measurement of pressures in the range from 10^2 Pa up to 10^4 Pa was calibrated with a new primary pressure standard realizing the Pascal via the gas density by means of the quantum-based refractometry. DUT2 is called transportable optical pressure standard (TOP) and is a transportable version of the primary stationary optical pressure standard (SOP). All three devices in this simulation are fictitious examples. However, emphasis was placed on making them as realistic as possible.

Currently, this new realization of the Pascal is in the focus of research and development, since it is very attractive within the context of the redefined SI as well as due to its practicability and wide potential (speed, size, accuracy). It is the subject of the EMPIR project 18SIB04: ‘QuantumPascal’ (QP) [1, 2].

To point out the likely benefit of the UDCC, expected improvements on the uncertainty budget of the used primary pressure standard are considered that are likely to be achieved during the next years as well as their impact on the uncertainty chain starting from the NMI leading to uncertainty improvements for end users.

This presentation has the aim to invite for an open discussion on how the DCC could provide an uncertainty budget that is updatable over time (UDCC) and therefore providing improvable uncertainties (shown in Fig. 1.) even without recalibrations, which will be ensured by automatic or retrievable updates accessible by everyone within the calibration chain, including the end users.

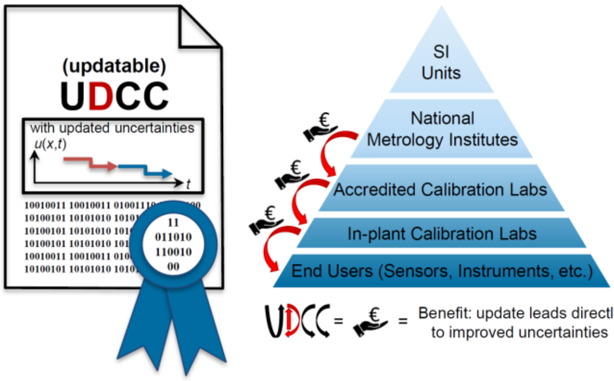

Fig. 1. Illustration of an updatable DCC (UDCC). As indicated by the graph, the uncertainties of the calibrated device might improve over time even without a recalibration.

2. MATERIAL AND METHODES

To point out the benefits of the UDCC a fictional refractometer will be considered for pressure assessments, with an uncertainty budget in accordance with the values in the recent literature [3]. In section 2.1. the working methodology is described in a simplified way and a few approximations in the model equation are assumed to focus on the essential. Details on the uncertainties of the refractometer-based primary standard and their expected improvements over the next years will be given in section 2.2. Section 2.3. will list the improvements assumed, that will have an influence on the uncertainty budgets followed by a short description of the CDG as the calibrated device under test in section 2.4.

2.1. Refractometry for pressure assessments

A simplified explanation of the pressure assessment utilizing a refractometer with a Fabry-Perot cavity (FPC) is given in the following text. When gas is introduced into the FPC-based resonator its resonance frequency ν_0 will change by Δf with respect to the refractivity $(n-1)$ of the gas as in equation (1).

$$(n-1) \approx \frac{\Delta f/\nu_0}{1+\frac{\Delta f}{\nu_0}+\varepsilon} \tag{1}$$

Here, ε describes the pressure-induced cavity deformation. Changes Δf in the frequency are typically assessed by a laser locked to the FPC by comparison to a frequency standard. Equation (1) is simplified to an approximation, so no mode jumps, mirror penetration depths or the influence of the Gouy phase are considered. A more detailed descriptions can be found here [4].

The molar density ρ can be calculated from the refractivity using the extended Lorentz–Lorenz equation.

$$\rho \approx \frac{2}{3A_R}(n-1)[b_{n-1}(n-1)], \tag{2}$$

where A_R and b_{n-1} are dynamic polarizability and a series expansion coefficient, respectively. The latter is given by $b_{n-1} = -(1+\frac{4B_R}{A_R^2})/6$. Here, B_R is the second refractivity virial coefficient from the Lorentz–Lorenz equation. Equation (2) is also an approximation, since higher order refractivity virials have been neglected, which is plausible for the given pressure range. Finally, the pressure p can be obtained for a given temperature T from the density as in equation (3).

$$p \approx RT\rho[1+B_\rho(T)\rho], \tag{3}$$

were R is the molar gas constant, and $B_\rho(T)$ is the second density virial coefficient. Equation (3) is also an approximation since the higher order density virials are not considered for simplicity.

2.2. Primary standard (SOP)

The primary standard chosen for this example is based on the stationary optical pressure standard (SOP) [3]. The FPC spacer is made from the nickel–iron alloy Invar. Therefore, besides the mirrors, all parts in contact with the gas are made from metal are expected to have no notable outgassing, hysteresis, or aging effects. Using the so-called GAMOR method, no drifts on a 100 s time scale or slower will influence the assessed pressure [5].

The pressure induced deformation, which is one of the major challenges, when using refractometry for the primary pressure assessment, will be determined by the so-called two-gas-method, using the difference in refractivity from helium and nitrogen [6].

Its temperature stabilisation, which is another major challenge, is realized by the utilization of gallium. Therefore, it has an excellent repeatability and long-term stability. This is the status considered for Dec. 2023 and will lead to the expanded uncertainty contributions u(SOP) given under a) in Table 1. This is the time within this simulation when the two devices under test are calibrated for the first time.

The descriptions of several likely future events assumed that will lead to an improved uncertainty budget of the primary pressure standard can be found in section 2.3. 'Improvements assumed'. The development of all uncertainties over time, driven by the events b) to e) are given in Table 1. Row e) implies a recalibration of the DUT, which for example could be well communicated by a 'ready for beneficial recalibration' status-update via the UDCC. Otherwise (without the recalibration of the DUT) the improvement in the given uncertainty of the UDCC will be less for the last event (row 'e', 'December 2025').

2.3. Improvements assumed

The assumed improvements including a better knowledge of the relevant gas parameters achieved by science and improvements with respect to a better characterization of the primary standard used, are described in the following and are summarized in Table 1:

b) Jun. 2024: The gas temperature during the pressure assessment with the primary standard realized by the fixpoint thermalization will be characterized extensively, like in [7] leading to $u(T)$ 26 ppm -> 4 ppm.

c) Dec. 2024: The uncertainty of the polarizability of the gas used will be decreased by ab-initio calculations in combination with experimental assessments, halving the direct uncertainty contribution (8 ppm to 4 ppm). Indirectly this also leads to a decreased uncertainty contribution of the pressure induced deformation (1.5 ppm to 0.5 ppm).

d) Jun. 2025: The uncertainties of the virials of the gas used will be decreased by ab-initio calculations in combination with experimental assessments. The contribution of the density virials improves (3 ppm to 0.5 ppm) as well as the contribution of the refractivity virials will improve (1.8 ppm to 0.5 ppm).

e) Dec. 2025: Update of the primary standard by using two laser frequencies simultaneously as well as helium, argon, and nitrogen. Additionally, a comparison to other primary refractometers is performed. All in all, leading to the following improvements of uncertainty contributions: Polarizability AR (4 ppm to 3 ppm), gas temperature T (4 ppm to 2 ppm), laser frequency ν (3 ppm to 0.5 ppm), pV-work (2 ppm to 0.2 ppm), gas purity r_{purity} (1 ppm to 0.5 ppm), residual pressure p_0 (5 mPa to 1 mPa), and outgassing and leaks (11 mPa to 1.5 mPa).

2.4. Calibrated device Nr. 1 (DUT1: CDG)

The first fictive device under test (DUT1) is a capacitance-diaphragm gauge (CDG). It is suitable as an exemplary DUT for several reasons: It is a commercially available and widely used pressure measuring device whose measuring principle provides excellent results in the range 1 Pa to 10^5 Pa. Usually, two decades within the given range are covered with one device. For this simulation we choose the range from 10^2 Pa up to 10^4 Pa. CDGs have been in use for decades in the vacuum laboratories of almost all NMIs and they are known to be suitable as transfer standards for intercomparisons.

Based on available experience and investigations [8], the inherent difficulty of distinguishing between the repeatability of the primary standard and the repeatability of the DUT can be overcome for this type of instrument. The following expression for the expanded measurement uncertainty should therefore refer purely to a CDG, like the one used for this example with a full-scale of 10 kPa: $u(p,CDG)$ = 10 mPa + 10 ppm. Here, the repeatability, the digitization of the measurement signal and the non-detectable scatter of the offset during the pressure measurement were considered.

2.5. Calibrated device Nr. 2 (DUT2: TOP)

The second fictive calibrated device is based on the transportable optical pressure standard (TOP) [3]. It is also made from Invar. Since it is used as a transfer standard, many uncertainty contributions effecting the SOP will not contribute here. It covers the same pressure range, as the primary standard with an expanded uncertainty contribution (k=2) given by repeatability of the assessment of the beat frequency (0.8 ppm) as well as the thermal stability (2 ppm), leading to: $u(p,\text{DUT2})$ = 2.2 ppm.

Table 1. Summary of improvements of the relative uncertainties over time (k=2). Numbers are given in ppm. The constant terms for the u(SOP) are 12.2 mPa for rows a-c) and 2.3 mPa for row d) and not shown here, as well as the constant terms for $u(p,\text{DUT1})$ with 10 mPa and $u(p,\text{DUT2})$ with less than 2 mPa.

Symbol	a) Dec. 23	b) Jun. 24	c) Dec. 24	d) Jun. 25	e) Dec. 25
T	26	4	4	4	2
AR	8	8	4	4	3
B$\rho(T)$	3	3	3	0.5	0.5
v	3	3	3	3	0.5
pV-work	2	2	2	2	0.2
B(n-1)	1.8	1.8	1.8	0.5	0.5
ε	1	1	0.5	0.5	0.5
r_{purity}	1.5	1.5	1.5	1.5	0.5
u(SOP)	**27.7**	**10.4**	**7.6**	**6.8**	**3.8**
$u(p,\text{DUT1})$	10	10	10	10	10
u(UDCC1)	**29.5**	**14.5**	**12.6**	**12.2**	**10.7**
$u(p,\text{DUT2})$	2	2	2	2	2
u(UDCC2)	**27.8**	**10.6**	**7.9**	**7.2**	**4.3**

3. RESULTS AND DISCUSSION

As explained in section 2, the simulated uncertainty budget of the exemplary primary standard will improve over time, leading also to improved uncertainties of the DUT. Usually, this benefit comes into play with a recalibration of the DUT. The proposed concept of the dynamic and thus updatable UDCC enables the benefit for the calibrated devices to occur already sooner. Fig. 2 is illustrating these improvements in uncertainties for all devices: the primary standard and the devices under test.

One point that would need to be addressed to make the UDCC work as intended is for example, under which conditions does the improved uncertainties count in fully with respect to the CMC. Key comparisons are not performed that often. So, for the given example a direct comparison of the primary refractometer to the best in-house piston gauges with an expanded uncertainty of $u(p)$ = 2 ppm (k=2, at 100 kPa) might be an option until the key comparison (e.g., in Dec. 2025) validates the uncertainties given there. However, the elaboration of a ready-made solution for this is outside the scope of this presentation since its aim is to open for discussions.

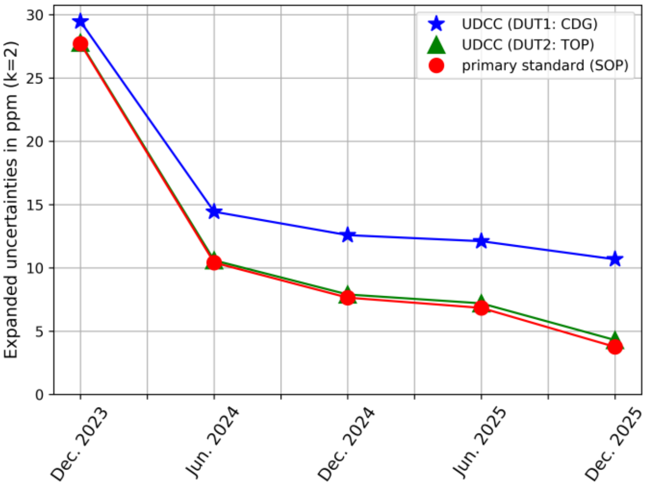

Fig. 2. Uncertainties in ppm (k=2) of the primary standard (SOP) in blue and in the updatable DCC (UDCC) of the two calibrated devices under test (DUT1 ‘blue star’ & DUT2 ‘green triangle’). The last points will only be achieved, when the DUTs are recalibrated, as explained in the text. All other updates improving the uncertainties will happen automatically.

4. CONCLUSIONS AND OUTLOOK

It was shown that for the two given examples the proposed functionality of an UDCC will bring direct benefits also to the end users, by decreasing the uncertainties even without recalibrations. It also shows that the UDCC enables for a new way to inform the end user about the benefits of a recalibration with an improved primary standard.

The DCC is new and there are many potential use cases that will benefit from it. Other examples would be reductions in the uncertainties between the ITS90 (temperature scale based on fixed points) and the thermodynamic temperature scale or the significant difference with respect to the realization of the kg utilizing a Silicon-sphere and a Kibble balance. E.g., the use of the Monte Carlo method with respect to supplement 2 of the ‘Guide to the Expression of Uncertainty in Measurement’ (GUM) could consider corelations very well, and therefore sometimes improve the uncertainty by more than thirty percent compared to an uncertainty budget based on supplement 1.

In order to take advantage of the UDCC-based benefits presented here, a corresponding implementation must be worked out. Exciting questions regarding possible implementations as well as their prerequisites and consequences open up. For example, how will the update reach the end user? A first step could be a ‘push notification’ that will be sent automatically to the owner of the DUT as soon as an update is achieved. The owner of the DUT could receive the updated DCC and thus change the original DCC to a historical one, that was just replaced by the updated one.

Far more visionary would be the possibility to include formulas and variables into the DCC itself. Then the variables could be linked to a repository entry owned and updated by the NMIs. An automated update would be possible to guaranty the newest and thus lowest uncertainties to the end user’s device, which at this time should be able to interpret its own UDCC. This presentation shows one possible benefit of many of the DCC - provided the way is paved for them.

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