Models for Digitalized Measurement Data

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Abstract: Metrology's digital transformation continues to progress. The NCSL International 141 MII and Automation Committee recently emphasized the importance of careful conceptualization and modeling while agilely implementing digitalized processes in order to instill value in digital transformation. To this end, the committee sponsored a seminar at the 2024 NCSLI Workshop and Symposium with the theme "Conceptualize, Model and Implement". In this paper we review the committee's long-standing model for measurands in digitalized accreditation scopes to refine and extend that model to measurement data appropriate for interoperable use in instrument specifications and calibration certificates. Whether digitalized metrology organizations ultimately exchange that information in the form of complete documents that mimic current practices or via some as-yet-undetermined innovation, such data underlie all metrology operations and therefore require thorough modeling. We propose open-source models suitable for implementation in any exchange format (JSON, XML, etc.) and encourage industry collaboration to further refine the models.

Learning objectives

The presentation and paper address these topics:

1. Measurement-Information Infrastructure (MII);
2. Process and information modeling concepts;
3. Interoperable and reusable measurement data.

Learning outcomes

Those who see the presentation and read the paper should gain

1. a big-picture view of NCSLI's digital-transformation efforts;
2. some appreciation for conceptual models and their applications in digital transformation;
3. a glimpse of the business value in digitalized measurement data.

1. Introduction

Like any other reality-based industry, metrology operates on a cost-benefit relation and thrives only to the extent that it provides customers a positive net value. Other modern endeavors—finance, B2B, online retail, travel, entertainment, media—have leveraged digital transformation (DX) in order to provide new and greater value at lower cost. Our industry has embarked on DX with all the requisite resources: consensus standards, plentiful computing power, laboratory and enterprise management software, automated measurement systems and a huge alphabet soup of applicable information technologies. Despite these resources and many years of interest and development, we have not yet achieved DX in metrology.

Other industries have succeeded at DX by carefully abstracting their processes and data flows, modeling the supporting data and then applying standardized technology solutions to implement those models in digital systems. In metrology, our processes revolve around measurement descriptions, measurements and the resulting measurement data and quality thereof. The data doesn't sit ignored; calibration laboratories, testing laboratories, inspection bodies, instrument manufacturers, ABs[1], scientific organizations and others exchange the data in vast quantities throughout the measurement economy. To digitally transform metrology, we should therefore design, adopt and apply a common conceptual model for exchanging digitalized measurement data.

2. Costs and benefits

Conceptual models, however, do not appear magically but rather require much careful abstract thought and refinement—an up-front cost that we should expect to recover. The modeling process should consider all known process and feature variants within the target arena's scope. The resulting abstract model then includes mathematical relations and data structures that will represent any concrete instance within scope. An abstract conceptualization of a bird, for instance, should consider the concrete variants among bird species in flying, feeding, calling, mating, migration and other activities as well as variants in concrete features such as colors, sizes, shapes, feathers, . . . , and therefore capture sufficient data to represent any actual bird.

2.1. Costs

The modeling approach does introduce some disadvantages beyond the up-front cost. We should acknowledge, for example, that comprehensive modeling delays DX implementation and any expected revenue or savings. If we mainly wanted to digitalize a penguin we wouldn't want to spend time modeling a general flying process for birds. Likewise, the Physikalisch-Technische Bundesanstalt and its partners pursued a development strategy for the DCC[2] [1] that focused on quick implementation of the most prevalent measurement cases rather than attempting to model the general case up front. This approach has generated much interest in metrology's DX and many implementation efforts worldwide.

Proceeding without a suitable model has a long-term cost though: The implementation may fragment into separate cases that do not integrate well. Without an overall conceptual model that structures and identifies the data, we sacrifice interoperability—our systems will not recognize and process the data autonomously and thus still require the manual intervention (labor costs) we would like to eliminate. If, for example, the measurement-data structure for pressure differs from that of voltage, length or radiance, those multiple disjoint cases quickly burden software implementations, a significant development and maintenance cost that every software developer will suffer. Since we already expect to ultimately transform the entire

[1]accreditation body

[2]digital calibration certificate

IQI[3]—all measurement processes and quantities—it makes sense to model measurements generally, abstractly, from the start and to expect a higher return.

Another cost consideration involves the tooling or lack thereof to (at least help) transform conceptual models into actual implementations. Ideally, designers have fit-for-purpose tooling to digitally produce a conceptual model from which the tooling will produce data models for any chosen software development system. Development systems would take the data models and construct all the essential code for incorporating the model into an application. Pieces of that tool chain already exist for various development ecosystems: model-driven architecture [2], model-driven software engineering [3], object relational modeling [4], model-view-controller technology, LLMs[4] customized for software-development assistance. Implementers may also build their own tools for repeated use to fill the gaps.

2.2. Benefits

We expect net positive value from conceptual modeling, benefits that exceed costs. As one benefit, conceptual modeling bakes in no particular implementation technology. This agnosticism leaves developers free to independently choose their computing platform, local data-storage method and data-exchange formats. For example, an application may store its data in any desired database format and then serialize-deserialize it per the conceptual model to-from XML[5], JSON[6] or any other data standard. Existing information technology has long since made this trivial.

As a key benefit, conceptual modeling should provide interoperability as implied in Section 2.1. Digital interoperability and reusability mirrors objectivity in human communication [5]. Both require source-independent semantic meaning and validity, which means

1. correct reasoning—well designed data & process models for the present and future,
2. data transformed to a standardized context—reference metadata and unique identifiers,
3. correct formulation—standardized meanings, (linked) definitions, controlled syntax;

and freedom from subjectivity such as

1. arbitrariness—undefined or free-form data fields,
2. ambiguity—multipurpose data fields, missing unique identifiers, unclear definitions,
3. out-of-context placement—essential elements falling outside the modeled framework.

The IQI operates as an economy in which entities produce and consume measurement data [6]. A digital IQI economy requires data interoperability, which in turn requires well reasoned conceptual models.

That measurement-data interoperability facilitates software innovations that will bolster the bottom line by realizing DX's potential value. We list here some services machines might

[3]international quality infrastructure
[4]large language models
[5]eXtensible markup language
[6]JavaScript object notation

perform that people currently either avoid or expend excess labor on.

- Locate and rank all laboratories with the capabilities to calibrate a given instrument or inventory.
- Locate and rank all instruments on the market that will meet an application's measurement requirements.
- Calculate point-by-point CMC[7] uncertainties and MPEs[8] on the fly.
- Generate customized instrument specifications or DCRs[9] and issue purchase orders.
- Generate CMCs from instrument specifications and calibration certificates.
- Optimize instrument specifications or calibration intervals from calibration history.
- Generate automated, customized calibration procedures from instrument specs, DCRs and calibration certificates.
- Improve uncertainty estimates flowing through the traceability network.
- Recover lost value from over-simplified MPEs, CMCs and measurement uncertainties [7].
- Validate certificate uncertainties against accreditation scopes [8].
- Verify received certificates' accreditation status and compliance to calibration requirements for each reported measurement.
- Verify an AB's ILAC[10] MRA[11] or an NMI's[12] CIPM[13] MRA status.
- Automate non-conformance investigations.
- Calculate uncertainty and other measurement-quality metrics between and beyond calibration points.
- Propagate calibration uncertainties to all dependent test & measurement processes.
- Correct all measurements for instrument bias (transparent adjustments).
- Facilitate digital twins and smart instruments.
- Streamline assessments and audits.
- Validate all data automatically at every step.

All these benefits stem from lowering the data-exchange hurtles between testing and calibration labs, instrument manufacturers, vendors, accreditation bodies and measurement

[7] calibration and measurement capability
[8] maximum permissible error
[9] digital calibration requests
[10] International Laboratory Accreditation Cooperation
[11] mutual-recognition agreement
[12] national metrology institute
[13] International Committee for Weights and Measures

consumers [9]. Innovators will expand this list far beyond what we might predict and the market will determine where the real value lies, but we should expect a large return from the up-front modeling investment.

3. Model requirements

Let's now examine, refine and build measurement-data models. For digitalized interoperability, we want to structure our model in such a way that machine will know what (measurands) an instrument measures, what measurements (measurands) we claim capabilities for and what (measurands) we measured in a calibration or other measurement service. In short, since measurement data revolve around the *measurand*, our model should do likewise.

What exactly does "measurand" mean? Rephrased, the VIM [10, 2.3] defines "measurand" as the quantity we intend to measure. In the definition's first note, the VIM adds that the measurand specification "requires knowledge" of the "quantity" kind and the "state of the phenomenon, body, or substance carrying the quantity". The VIM adds further in Note 3 that since the measurement, measuring system and measurement conditions might change the quantity under measurement, the measurement requires adequate correction in order to match the defined measurand. (See the definition's EXAMPLEs.) All together this means we should unambiguously define the measurand, with a perfection commensurate with the uncertainty desired, by specifying the measured quantity [10, 2.10], its influence quantities [10, 2.52], relevant properties [10, 1.30] and operating conditions [10, 4.11].

Without that qualifying information, the measurand's definitional uncertainty [10, 2.27] may nullify the measurement's value. In today's IQI, the lack of such detail often causes errors and misunderstandings when procuring and performing measurement services, resulting in either protracted conversations to determine the actual measurement desired, measuring the wrong measurand, or both. To expect machines to interpret the measurand correctly without that manual intervention therefore requires an unambiguous measurand specification with sufficient definitional detail to support the desired uncertainty.

To support any desired uncertainty the model should allow unlimited, exacting measurand qualifiers and allow their omission when insignificant relative to the measurement uncertainty or irrelevant to the service procured; in other words, we want an unambiguous abstract model flexible enough to handle any circumstance and one which anyone may instantiate with only the detail that matters for a particular concrete application.

Note also that the VIM measurand definition says nothing about any particular measurand, measurement field, quantity, etc.; the definition applies to *all* measurement types without any special exceptions or additional concepts for particular measurements. We therefore infer that we may indeed create a *universal* conceptual model for measurement data that will handle any concrete instance.

4. The measurand model

Some time ago, the NCSL International 141 MII and Automation Committee [11] modeled measurement data abstractly [12–17], concretized it as an XML schema and applied it to digitalizing SoAs[14] [18–20]. The committee later established a repository of concrete measurands conforming to the model on GitHub [21] and recently began refining that model to prepare for a formal release. Figure 1 illustrates a refined, provisional measurand model, not yet considered in committee, that meets Section 3's requirements.

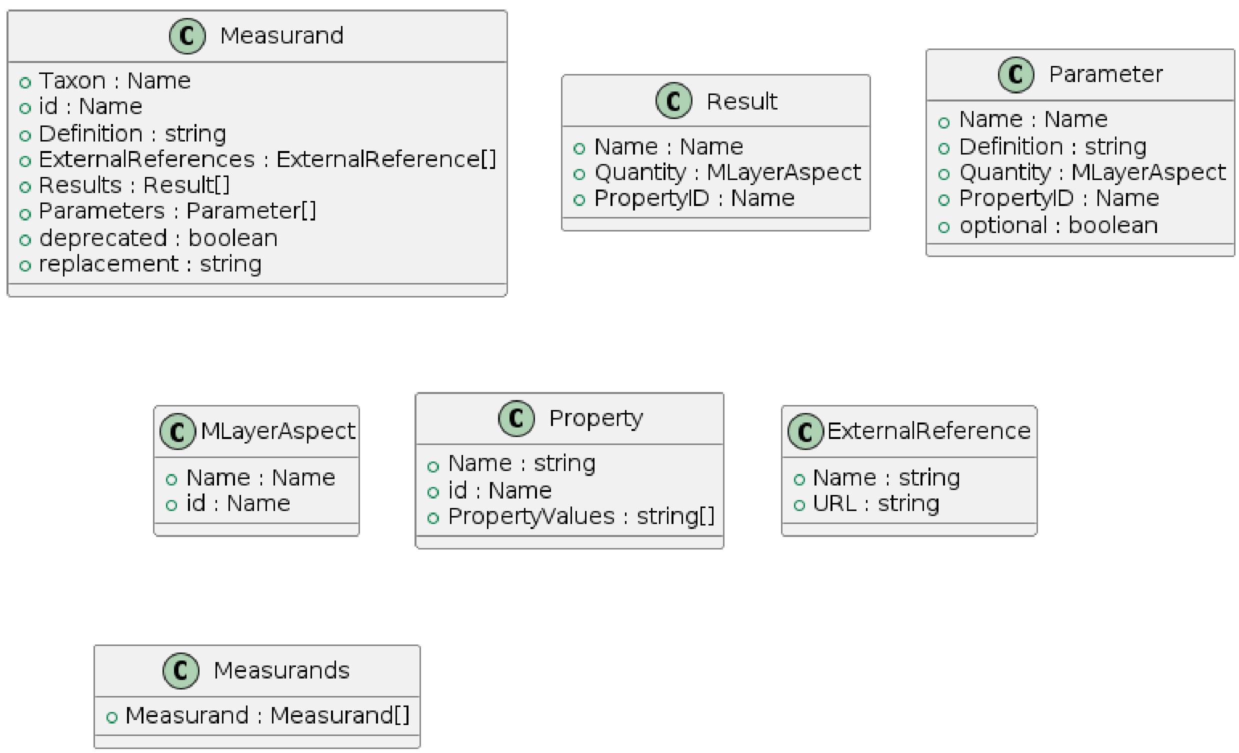

Figure 1. The provisional measurand model's essential elements. Element names differ from the current model [21].

The model in Figure 1 comprises seven entities. The main entity, the `Measurand` itself, contains a human-readable `Definition` for maintenance and manual applications along with any number of `ExternalReferences` to tie the measurand to authoritative references or definitions. The `ExternalReference` entity provides for a `Name`, e.g. "ISO/CIE 23539:2023" (photometry definitions), and a `URL` link to, say, a digitalized document's entry for that measurand or to another machine-readable endpoint. `ExternalReferences` may either replace or back up `Definition`.

More important for interoperability though, the `Taxon` metadata uniquely identifies the `Measurand`. Each taxon takes a defined form [22,23] such as `Source.Voltage.AC` and comes with a unique identifier `id` for linking to an external controlled list.

To complete our interoperability requirements, `Measurand` contains `Results`, which specifies in machine-readable form the measured quantity (or examined property), and zero or more `Parameters` to qualify the measurand. Each `Parameter` may also specify either a measured quantity or examined property. To unambiguously specify the `Quantity`, we use the M-

[14] accreditation scopes

layer [24, 25] and point to an `MLayerAspect` by its unique aspect `id`. We include the M-layer's aspect `Name` for easy maintenance. In the case of a property, we identify it by its controlled `PropertyID` and point to its `Name`, e.g. "ThermocoupleType" and a list of valid `PropertyValues`, e.g. "J", "K", "T", ...

For maintenance convenience, the `Result` entity includes a `Name` irrelevant to interoperability. The `Name` in the `Parameter` entity, however, plays an essential interoperability role. A measurand may have multiple parameters of the same quantity; for example, calibrating an amplifier's voltage gain involves both an input and output voltage. As Table 1 shows, `Name` distinguishes the two in order to properly match, for example, an instrument's input and output voltage ranges to a lab's capability for each without mixing them up.

Table 1. Matching parameters between different instantiations of an abstract measurand. The two measurands match, pending further evaluation of measuring intervals and uncertainty requirements.

Model Element	Instrument Measurand		CMC Measurand
`Measurand.Taxon`	"Source.Ratio.Voltage.AC"	⇔	"Measure.Ratio.Voltage.AC"
`Result.Name`	"Gain"	⇔	"Gain"
`Parameter.Name`	"Frequency"	⇔	"Frequency"
`Parameter.Name`	"InputVoltage"	⇔	"InputVoltage"
`Parameter.Name`	"OutputVoltage"	⇔	"OutputVoltage"
`Parameter.Name`	not used (optional)		"AmbientRH"

The `Parameters` specify all the relevant influence quantities, properties and operating conditions. Depending on context and required uncertainty, not every measurand requires every parameter in every instance. For example, sourcing an AC voltage requires knowing the frequency and only in some cases the ambient relative humidity. The `optional` element differentiates these cases for data validation. See Table 1.

Wrapping up the `Measurand` entity, `deprecated` and `replacement` help provide backward compatibility if replacing one measurand in the measurand taxonomy with another. The measurand model also includes other elements not discussed here: such non-essential niceties as measurement category and discipline, mappings to other quantity systems, etc.

Finally, the `Measurands` entity wraps up a set of measurands into a catalog.

5. Applied measurement-data models

Having a measurand model, we now build upon it to design models for actual application to digitalized measurement data. The committee originally envisioned models for three MII metrology documents: instrument specifications, SoAs and calibration certificates or testing certificates. We recognize that systems will store (and might exchange [26]) measurement data without a formal document wrapper but the three basic extended models still apply. At first glance each document type will add measurement data of differing types to the measurand model and thus requires its own measurement-data model variant. The following sections discuss each document's measurement data in turn.

5.1. Measurement specifications

We have little to test or calibrate or to claim capabilities for without instruments and their measurement specifications. We do of course test products, most of which do not constitute measuring instruments, but for our purposes we may consider a measurable product specification equivalent to an instrument specification. We may also consider the DCR a set of specifications derived from an instrument specification and augmented with business transaction data for procuring calibration services. A measurement-specification model therefore applies to instrument specifications, product specifications and DCRs.

The essential difference between a specification's measurement data and that of CMCs and measurement results: a specification includes a requirement, typically an MPE, which the VIM defines [10, 4.26] as "extreme value of measurement error . . . permitted by specifications or regulations for a given measurement, measuring instrument, or measuring system". Notice again the definition's universality—our model should again apply to any measurement.

MPEs typically come into play when we we verify instruments, but at higher traceability levels the requirement often comes as a maximum uncertainty for the measurement result. A DCR may in fact specify target uncertainties instead of MPEs, so we seem to have two separate cases to model. If, however, we recognize an MPE as a merely an expanded uncertainty commensurate with some coverage probability, then we might model both cases with the same abstraction. An interoperable instrument specification therefore boils down to a fully qualified measurand and an uncertainty specification.

5.2. Calibration and measurement capabilities

Given an instrument to calibrate and its specifications, we may devise measurement capabilities to address those calibration requirements. Whether published in the KCDB[15] under the CIPM MRA, on an SoA under the ILAC MRA, or simply listed as an unaccredited service, an interoperable CMC simply comprises a fully qualified measurand and a recognized or claimed uncertainty.

5.3. Measurement results

Finally, having measurement specifications and capabilities, we may produce a measurement result, which the VIM defines [10, 2.9] as a "set of quantity values being attributed to a measurand together with any other available relevant information". As the definition's NOTE 2 acknowledges, we typically represent a measurement result by a single measured quantity value and a measurement uncertainty. An interoperable measurement result therefore combines a fully qualified measurand and a measurement uncertainty. We consider further details in Section 5.4.

5.4. Comprehensive measurement-data model

To summarize the previous three sections, we do not require a separate model for each document type. Adding an uncertainty element to our measurand model should cover any measurement data:

1. instrument specification: fully qualified measurand and an uncertainty specification

[15] Key-Comparison Database

2. CMC: fully qualified measurand and a recognized or claimed uncertainty
3. measurement result: fully qualified measurand and a measurement uncertainty

Note the “fully qualified” in each description. We have fully qualified the measurand in the abstract but not for any concrete measurement data—we ignored certain excerpts in the VIM definitions for MPE (“with respect to a known reference quantity value”) and measurement result (“set of quantity values”). Concrete MPEs, measurement results and CMCs all specify quantity values or ranges (measuring intervals [10, 4.7]). In the simplest case this just means associating a number and M-layer scale (unit) with the already given M-layer aspect. One such construction for each endpoint together specify a range of values for a CMC or instrument function and collapse to a single point when equal. The existing SoA schema [19] took this tack but lacked the M-layer.

Anticipating DX benefits though, we should take a wider view and look for a more complete abstraction. To leverage machine power and extract the most DX value, metrological data models should incorporate mathematical expressions wherever appropriate [7]. As with many higher-level model elements [7] beyond this paper’s scope, mathematical expressions would represent quantities—values and ranges—more generally. Valid expressions would include any number (x), an equation explicitly tying a quantity symbol to the number ($q = x$) or a range ($L \leq q < H$) between the numbers L and H, inclusively (L) or exclusively (H). Expressions would also handle more complicated relations such as $L \leq Vf \leq H$, where Vf represents a voltage-frequency product of two parameters, or $V_1 < V_2 < 2V_1$, where one parameter’s allowed range depends on another. Based on the immense flexibility provided, we update our model to use expressions for all quantity values.

For a property parameter, we simply express a concrete value as a list of one or more of the allowed values that the abstract measurand defines. An examination would likely result in a single value, whereas a CMC or specification might include multiple values to express the laboratory capability or instrument function.

Figure 2 illustrates those elements of the resulting provisional measurand model for concrete measurement data that differ from Figure 1. The `Result` and `Parameter` each add four new elements: `Symbol`, `QuantityValues`, `Uncertainty` and `PropertyValues`. `PropertyValues`, when applicable, simply lists the measurement data’s concrete values.

We structure `QuantityValues` per the new element `AspectValues`, which identifies the quantity by its M-layer `AspectID`, the unit by its M-layer `ScaleID` [25], and the numeric values by a (perhaps symbolic) mathematical `Expression` that a machine will resolve. Here we show the `Expression`’s (pseudo-) data type as `Math`. MathML[16] [27] would work here but that assumes an XML data format, so the abstract element simply amounts to math. `Symbol`, unique within a given measurand, also encoded as `Math`, constitutes metadata that ties a variable name to `Result` and each `Parameter` so that all `Expression`s may reference them uniquely.

We may classify measurement data in another dimension besides the CMC-MPE-measurement

[16] mathematics markup language—content markup in particular, not simply presentation markup, so that it remains machine-actionable

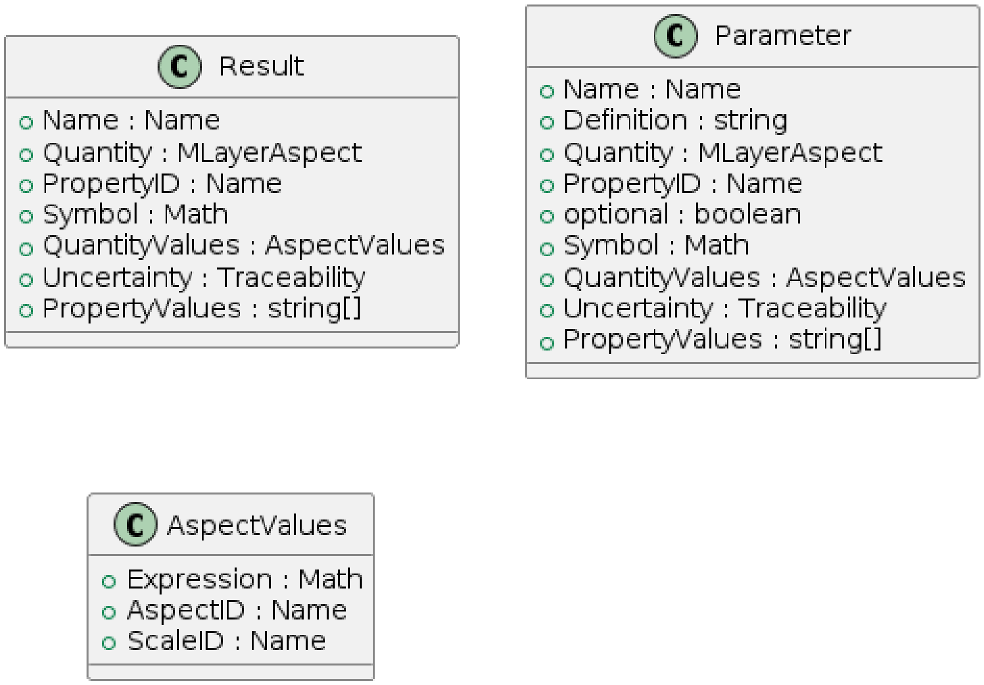

Figure 2. The provisional model's modifications for concrete measurement data. Element names differ from the current model [21]. Non-essential data elements not shown.

result categorization. Namely, we have nominal values, reference values, measured values, error values, corrections, etc. Measurement ranges appear as nominal indication intervals (named range: $\pm$ (0 mV to 200 mV)), actual indication intervals (physical range: $\pm$ (0.0 mV to 199.9 mV)), and certified measuring intervals (calibrated range: $\pm$ (10.0 mV to 199.9 mV)). For a given measurement datum, the same measurand covers all these variations and so we would simply repeat the quantity values as desired under the same umbrella, giving each an appropriate metadata tag. The same applies if we would like to include verification data (an MPE) in a calibration certificate along with the measurement data.

Notice that we have left the `Traceability` element undefined. The committee's existing SoA schema [19,20] uses a complex structure to represent CMC uncertainties as calculable expressions but we anticipate moving to a much more general structure. The new structure should of course also handle specifications and measurement results. It should also allow for simple uncertainty expressions and various uncertainty representations and propagation methods, including a representation of the entire traceability network leading to the uncertainty of interest [2].

Note that Section 3's model requirements did not include input quantities as a parameter type. While a particular parameter may double as an input quantity for a particular measurement method, input quantities only arise in the context of uncertainty estimation, so we expect the uncertainty model to reuse the measurand model to represent input quantities.

One might question why we would include such a comprehensive uncertainty model in CMCs and MPEs. A structured, quantified traceability model supports not only calibration results, but also CMC uncertainties (with worst-case estimates for some error sources) and MPEs (with error sources from drift and operating conditions). So in a DX context, an embedded traceability chain would empower machines with the data to document the provenance [28] and derivations of our stated CMCs and MPEs, thus facilitating assessments, maintenance and refinements [5].

The requisite uncertainty structures already exist in particular implementations [29–32] but we await a technology-agnostic conception that covers all current and envisioned practices. Though lacking certain refinements, that completes this stage of our comprehensive measurement-data model.

6. Conclusion

A common conceptual model for exchanging digitalized measurement data will power metrology's digital transformation. Standardized reference metadata sets with a universal reference model for measurement data will facilitate the application software that will streamline our international quality infrastructure by providing interoperability. This paper illustrates such a model that, though a work in progress and not final by any means, suffices to start using the measurand taxonomy to identify and exchange interoperable data. Few first-version models will capture every real-world case that arises, but agile iterations of the conceptualize-model-implement process will drive success.

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