CEN WORKSHOP AGREEMENT

CWA 17815

January 2025

ICS 01.040.07; 07.120; 17.020

Supersedes CWA 17815:2021

English version

Materials characterization - Terminology and structured documentation

This CEN Workshop Agreement has been drafted and approved by a Workshop of representatives of interested parties, the constitution of which is indicated in the foreword of this Workshop Agreement.

The formal process followed by the Workshop in the development of this Workshop Agreement has been endorsed by the National Members of CEN but neither the National Members of CEN nor the CEN-CENELEC Management Centre can be held accountable for the technical content of this CEN Workshop Agreement or possible conflicts with standards or legislation.

This CEN Workshop Agreement can in no way be held as being an official standard developed by CEN and its Members.

This CEN Workshop Agreement is publicly available as a reference document from the CEN Members National Standard Bodies.

CEN members are the national standards bodies of Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Republic of North Macedonia, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Türkiye and United Kingdom.

EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

CEN-CENELEC Management Centre: Rue de la Science 23, B-1040 Brussels

Ref. No.:CWA 17815:2025 E

Contents

Page

Foreword

This CEN Workshop Agreement (CWA 17815:2025) has been developed in accordance with the CEN-CENELEC Guide 29 “CEN/CENELEC Workshop Agreements – A rapid way to standardization” and with the relevant provisions of CEN/CENELEC Internal Regulations - Part 2. It was approved by the Workshop CEN “Materials characterisation - Terminology, metadata and classification”, the secretariat of which is held by UNI, consisting of representatives of interested parties on 2024-12-04, the constitution of which was supported by CEN following the public call for participation made on 2024-04-21. However, this CEN Workshop Agreement does not necessarily include all relevant stakeholders.

The final text of this CEN Workshop Agreement was provided to CEN for publication on 2024-12-16.

Results incorporated in this CWA received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 952869.

This document supersedes CWA 17815:2021.

The following organisations and individuals developed and approved this CEN Workshop Agreement:

— GOLDBECK Gerhard (Chair) – Goldbeck Consulting Ltd

— PIA Chiara (Secretary) – UNI

— AL-ZUBAIDI R-SMITH Nawfal – Keysight Technologies GmbH

— BIAGINI Davide – Technical University of Delft

— BLEKEN Francesca Lønstad – Sintef

— BORRAS Xavier – i-TRIBOMAT: The European Tribology Centre

— CAPRIA Ennio Tito – ESRF

— CHARITIDIS Costas – National Technical University of Athens

— CLAUSNER André – Fraunhofer-Institut für Keramische Technologien und Systeme

— DE BAAS Anne F. – AnneFdeBaas Materials Research

— DE MARCHI Julian – Royal Netherlands Aerospace Centre

— DEL NOSTRO Pierluigi – Goldbeck Consulting Ltd

— EXNER Thomas E. – Seven Past Nine GmbH

— FRIIS Jesper – Sintef

— GRUNEWALD Christian – DIN Deutsches Institut für Normung

— HELM Dirk – Fraunhofer IWM

— HORSCH Martin Thomas – Norwegian University of Life Sciences

— JOSHI Devendra – TEMAS Solutions GmbH

- KOUMOULOS Elias – IRES Innovation in Research and Engineering Solutions
- KRÖLL Mirco – Bundesanstalt für Materialforschung und -prüfung (BAM)
- KUMARASWAMY Kiran – Fraunhofer IWM
- LÓPEZ-QUILES PASTOR Javier – UNE Spanish Association for Standardisation
- MONTICELI Francisco –Technical University of Delft
- MOREL Elise – TEMAS Solutions Gmbh
- NAHSHON Yoav – Fraunhofer IWM
- OLIVIERI Federico – National Research Council
- ORFANIDIS Savvas – National Technical University of Athens
- PACE Maria Lucia – Consiglio Nazionale delle Ricerche
- PFEILER Olivia – KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH
- PORTELLA Pedro – Fraunhofer-Institut für Werkstoffmechanik IWM
- RASHID Saqib – Università degli Studi Roma Tre
- ROSSI Edoardo – Università degli Studi Roma Tre
- SABETTA Annamaria – National Research Council
- SANTAGATA Antonio – Consiglio Nazionale delle Ricerche
- SCHÖNHOF Raoul – HS Booster
- SEBASTIANI Marco – Università degli studi Roma Tre
- SIMPERLER Alexandra – Goldbeck Consulting Ltd
- TSATSOULIS Theodoros – National Technical University of Athens

Attention is drawn to the possibility that some elements of this document may be subject to patent rights. CEN-CENELEC policy on patent rights is described in CEN-CENELEC Guide 8 "Guidelines for Implementation of the Common IPR Policy on Patent". CEN shall not be held responsible for identifying any or all such patent rights.

Although the Workshop parties have made every effort to ensure the reliability and accuracy of technical and non-technical descriptions, the Workshop is not able to guarantee, explicitly or implicitly, the correctness of this document. Anyone who applies this CEN Workshop Agreement shall be aware that neither the Workshop, nor CEN, can be held liable for damages or losses of any kind whatsoever. The use of this CEN Workshop Agreement does not relieve users of their responsibility for their own actions, and they apply this document at their own risk. The CEN Workshop Agreement should not be construed as legal advice authoritatively endorsed by CEN/CENELEC.

Introduction

Standardisation is relevant for an integrated technological development. Particularly, early standardisation of terminology has been identified as useful to European research projects and important in establishing the European Research Area (ERA) as well as a European single market for goods and services.

A standardised, generalised terminology and structured documentation improves future exchanges in the entire area of materials characterisation. It has the potential to foster dialogue and mutual understanding between all stakeholders in materials characterisation, such as experts in characterisation techniques, operators and users of characterisation in academia, industry and instrument manufacturers, and developers of software used for data mining and AI model training. The structured documentation proposed in this CWA aims to support FAIR data[1], improve traceability and reproducibility of materials characterisation procedures, and hence interpretation and reliability of the resulting materials data. Furthermore, it is expected to ease the barrier to utilising increasingly powerful yet complex materials characterisation protocols for industrial applications.

The previous version of CWA 17815:2021 presented standardised schemas to describe the workflow of a given materials characterisation method by using the Materials CHAracterisation DAta (CHADA) documentation concept. The current version of CWA 17815 describes a more general workflow that is understandable by humans and supports machine-processable implementations. The adoption of a standard graphical notation, for instance the “Business Process Model and Notation” (BPMN[2]), is new in this version.

Also, since the previous version, the terminology and classification has been formalised into a taxonomy and an ontology of materials characterisation, called CHAMEO[3], which has in turn been used to inform the current CWA. The terminology used in CHAMEO also informs the interpretation of terms of this document[4]. These developments aim to support efficient solutions for documenting materials characterisation, enhance the communication, dissemination, storage, retrieval, and mining of data about materials characterisation, and contribute to efforts for materials taxonomy digitalisation.

---

[1] Go Fair, https://www.go-fair.org/

[2] Object Management Group Business Process Model and Notation, https://www.bpmn.org/

[3] Characterisation Methodology Domain Ontology (CHAMEO), https://github.com/emmo-repo/domain-characterisation-methodology

[4] Module: Characterisation Methodology Ontology, https://emmo-repo.github.io/domain-characterisation-methodology/chameo.html

1 Scope

The objective of this CWA is to provide a standard set of concepts, metadata and terminology that form the basis for documentation of materials characterisation. Its aim is to cover the most wide-ranging interpretation of “materials characterisation”, including the whole range of processes by which the structure and properties of a material, or even a system of materials, are ascertained. It includes any materials analysis process including macroscopic techniques. Also, the related field of materials testing is likely to benefit from this standardised documentation.

The CHADA starts with documenting the context and the rationale for the specific characterisation to be undertaken. For example, the performance of a candidate material (or combination of materials) for a given application could be determined by the appreciation of different material properties. Following that, the CHADA documents the material or materials systems under investigation and the sample(s) that are tested. Subsequently, the characterisation workflow is documented, covering all possible experimental and data processing workflow stages (with tables for each stage) until the aggregated outcome. The overall workflow consists of a combination of different workflow stages executed consecutively or in parallel.

The modular approach provides flexibility to repeat or skip stages depending on the case to be documented. If necessary, attributes of entities can be added, extended, or otherwise enriched to describe their properties and specifications at the desired level of detail related to the domain of academic or industrial expertise, and the intended scope or application.

Time series, multiple probes/samples and multi-materials cases (such as systems) can be documented by interpreting each concept to represent a list/series (that is, an array). By using the material and sample entity as an array representing several materials in a system, the CHADA can be applied to the documentation of the characterisation of materials systems, that is, systems of interacting materials (for example, tribological characterisations, structural health monitoring, component tests).

The output of a characterisation workflow can be either qualitative, semi-quantitative or quantitative. Finally, the outcome, which is the digestion and/or interpretation of the characterisation output(s), is presented.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardisation at the following addresses:

— ISO Online browsing platform: available at http://www.iso.org/obp/

— IEC Electropedia: available at http://www.electropedia.org/

3.1
batch
specific quantity of material produced or processed at one time, under the same conditions

Note 1 to entry The term batch is often used in manufacturing and production industries to track, control, and ensure the quality of materials. Each batch typically has a unique identifier and may be subject to quality control measures to ensure consistency and compliance with quality standards.

3.2
calibration data
output data of a measurement on a reference sample by a specific measuring instrument/device/system

Note 1 to entry Calibration data are post-processed into corrections to be used to correct measured characterisation data or to perform uncertainty calculations.

3.3
calibration process
operations/actions under specified conditions that are needed to obtain the correction used to convert the signal of the characterisation measurement (as produced by the detector) into the raw characterisation data

EXAMPLE 1 In nanoindentation, the electrical signal coming from capacitive displacement gauge is converted into a calibrated raw-displacement data.

EXAMPLE 2 In nanoindentation, the electrical signal coming from capacitive displacement gauge is converted into a real raw-displacement signal after using a proper calibration function (as obtained by the equipment manufacturer). Then, additional calibration procedures are applied to define the point of initial contact and to correct for instrument compliance, thermal drift, and indenter area function to obtain the real usable displacement data.

Note 1 to entry Within this workflow, a possible way is to use a reference sample (with pre-defined, specific, and stable physical characteristics and known properties) for the interaction with the measurement probe, in order to extract characterisation data to be compared to predefined values. In this way, the accuracy of the measurement tool and its components (for example the probe) is evaluated and confirmed.

3.4
Materials CHAracterisation DAta documentation (CHADA)
set of forms that document materials characterisation

3.5
characterisation data filtering
in data processing, process on a dataset to exclude, rearrange, or apportion data according to certain criteria

Note 1 to entry Preprocessing of raw data (for example, compacting data, removing outliers, filtering noise, interpolating missing data) is one type of characterisation data filtering.

Note 2 to entry The processing can include hardware filters (such as low pass filters "hardwired" to the sensor/probe).

3.6
characterisation data post-processing
data analysis and transformation that allows to calculate the material property/behaviour from the calibrated primary data

Note 1 to entry Characterisation data post-processing involves the application of a method, based on some theory or model, to primary data to calculate the secondary data that provide the information about the characterisation property or behaviour.

Note 2 to entry Characterisation data post-processing includes digital image processing to enhance or extract useful information.

EXAMPLE 1 In nanoindentation testing, the Oliver-Pharr method is used, which allows calculating the elastic modulus and hardness of the sample by using the load and depth measured signals.

EXAMPLE 2 Analysis of Scanning Electron Microscopy (SEM) (or optical) images to gain additional information, for example microstructural analysis, grain size evaluation, digital image correlation procedures.

3.7
characterisation data processing through calibration
process that describes how signal data are corrected and/or modified based on calibrations into raw data

3.8
characterisation experiment
execution of one specific characterisation workflow

Note 1 to entry The term “test case” is typically used for a characterisation experiment carried out to assess quality or performance against a defined reference or standard.

3.9
characterisation instrument
device used for executing characterisation actions to characterise a material, alone or in conjunction with one or more supplementary devices

3.10
characterisation laboratory
laboratory where a whole process or some of its stages take place

3.11
characterisation measurement process
process of experimentally obtaining data (values) that are attributed to a sample

3.12
characterisation outcome
digestion and/or judgement of the output of one or several tests given as feedback to the owner of the user story

3.13
characterisation primary data
data resulting from applying corrections to normalise and/or harmonise characterisation raw data, in order to prepare them for post-processing

3.14
characterisation raw data
output data of the characterisation measurement given by the measuring instrument.

3.15
characterisation secondary data
data resulting from the application of characterisation data post-processing

Note 1 to entry Characterisation secondary data may represent a property or a behaviour.

Note 2 to entry Characterisation secondary data may be used to establish a materials relation for a simulation model.

3.16
characterisation signal
result (effect) of the interaction between the sample and the probe or between the samples, which usually is a measurable and quantifiable quantity

Note 1 to entry Characterisation signal is usually emitted from a characteristic “emission” volume, which can be different from the sample/probe “interaction” volume and can be usually quantified using proper physics equations and/or modelling of the interaction mechanisms.

Note 2 to entry According to IUPAC Compendium of Chemical Terminology, a “signal” is “A representation of a quantity within an analytical instrument”.

3.17
characterisation workflow
process composed of all necessary steps (for example, sample preparation, calibration, measurement, post-processing) to establish the property, behaviour or image of a material or materials system

3.18
data pre-processing
process of curation (or preparing) data, which may come from disparate data sources, to improve their quality or reduce bias in subsequent analysis

Note 1 to entry If this process is applied to characterisation the input is raw data and the output is primary data.

3.19
data processing
computation that provides a data output following the elaboration of some input data, using a data processing application possibly exploiting a data processing model

3.20
detector
physical device (or chain of devices) that is used to measure, quantify and store the signal generated by interaction of the probe with the sample

EXAMPLE 1 Back Scattered Electrons (BSE) and Secondary Electrons (SE) detectors for SEM.

EXAMPLE 2 Displacement and force sensors for mechanical testing.

3.21
environment
surrounding medium

EXAMPLE 1 Environment of the material or materials system that appear(s) in the user story.

EXAMPLE 2 Medium that surrounds the characterisation sample in the experiment.

3.22
hazard
set of inherent properties of a substance, mixture of substances, or a process involving substances that, under production, usage, or disposal conditions, make it capable of causing adverse effects to organisms or the environment, depending on the degree of exposure (that is, a source of danger)

3.23
interaction volume
volume of material, and the surrounding environment, that interact with the probe or samples and generate a detectable (measurable) signal (information)

Note 1 to entry In some cases, the volume of interaction could be different from the volume of detectable signal emission. For example, in SEM, the volume of interaction between the electron probe and the material is different from the volumes that generate the captured signal.

EXAMPLE 1 In x-ray diffraction, the interaction volume is the volume of material that interacts directly with the x-ray beam and is usually smaller than the volume of the entire sample. Depending on sample's structure and microstructure, the interaction between the sample and the x-ray incident beam generates a secondary (reflected) beam that is measured by a detector and contains information on certain sample's properties (for example, crystallographic structure, phase composition, grain size, residual stress).

EXAMPLE 2 In SEM, the interaction volume is the volume of material that directly interacts with the incident electron beam, it is usually much smaller than the entire specimen's volume and can be computed by using proper models. The interaction between the scanning probe and the sample generates a series of detectable signals (for example back scattered electrons, secondary electrons, x-rays, specimen current) which contain information on, for example, sample morphology, microstructure, and composition.

3.24
level of automation
degree to which tasks are executed by machines using a specified protocol

3.25
level of expertise
specific experience, education, training and/or certifications required to carry out a task

Note 1 to entry This field is typically relevant only for materials testing in regulated environments.

Note 2 to entry The level of expertise in the CHADA may just be specified as low/medium/high or in a more detailed way with respect, for example, to operator qualifications or certifications for certain test techniques.

3.26
materials system
two or more materials that are in contact and/or interacting.

EXAMPLE Tribological properties (such as friction and wear) are not properties of a material, but properties of a system of two or more interacting bodies (for example, samples or components interacting with test probes or interfacial surfaces, non-destructive testing of machine components, inspection of materials in manufacturing processes). Consequently, multiple materials might be involved (for example, a polymeric and a metallic sample moving in a lubricated contact, or a sample subjected to chemical treatment).

3.27
measurement parameters adjustment
set of operations carried out on a characterisation measurement system using a sample which is not a reference sample so that it provides values considered to be correct for a quantity being measured

Note 1 to entry Adjustment of a measuring system is different to calibration, which is sometimes a prerequisite for adjustment. Adjusting/tuning a measuring instrument is an activity without a reference sample (which would be a calibration). The output of this process can be a specific measurement parameter to be used in the characterisation measurement process.

Note 2 to entry After an adjustment of a measuring system, the measuring system is usually recalibrated.

3.28
measurement uncertainty calculation
in data processing, the determination of the statistical dispersion of the values attributed to a measured quantity

3.29
operator
human person who takes care of the entire process or any of its sub-processes/stages, including operating the test equipment

3.30
probe
physical device or radiation (matter or field, together called a physical) that interacts with the sample and generates a response called signal

Note 1 to entry The probe is used to acquire information on the specimen's behaviour and properties.

Note 2 to entry In tribological characterisation and other techniques that investigate systems, a probe may be hard to define.

EXAMPLE 1 In x-ray diffraction, the probe is a beam of x-rays with known energy that is properly focused on the sample's surface with a well-defined geometry.

EXAMPLE 2 In electron microscopy (SEM or TEM), the probe is a beam of electrons with known energy that is focused (and scanned) on the sample's surface with a well-defined beam-size and scanning algorithm.

EXAMPLE 3 In mechanical testing, the probe is a force actuator that is designed to apply a force over-time on a sample. Many variants can be defined depending on way the force is applied (for example, tensile/compressive uniaxial tests, bending test, indentation test) and its variation with time (for example, static tests, dynamic/cyclic tests, impact tests).

EXAMPLE 4 In dynamic light scattering, temporal fluctuations of backscattered light due to Brownian motion and flow of nanoparticles are the probe, resolved as function of pathlength in the sample. From fluctuation analysis (intensity correlations) and the wavelength of light in the medium, the (distribution of) diffusion coefficient(s) can be measured during flow. The Stokes-Einstein relation yields the particle size characteristics.

EXAMPLE 5 In spectroscopic methods, the probe is a beam of light with pre-defined energy (for example in the case of laser beam for Raman measurements) or pre-defined polarisation (for example in the case of light beam for Spectroscopic Ellipsometry methods), that is properly focused on the sample's surface with a well-defined geometry (specific angle of incidence).

3.31
raw data normalisation
data processing which involves adjusting raw data to a notionally common scale

Note 1 to entry It involves the creation of shifted and/or scaled versions of the values to allow post-processing in a way that eliminates the effects of influences on subsequent properties extraction.

Note 2 to entry Raw data normalisation is one type of preprocessing of raw data.

3.32
reference sample
sample that is sufficiently homogeneous and stable with reference to one or more specified property(ies), which has been established to be fit for its intended referencing use in measurement or in examination

3.33
sample
portion of the material or materials system selected for characterisation or testing

Note 1 to entry The term 'sample' implies the existence of a sampling error, that is, the results obtained on the portions taken are only estimates of the property/behaviour present in the parent material.

Note 2 to entry Typically, the term is further qualified, for example, bulk sample, representative sample, primary sample, bulked sample, test sample.

Note 3 to entry An alternate term is specimen. Sample and specimen are sometimes used interchangeably, or also with slightly different meanings.

Note 4 to entry In fields such as composites, the term coupon is used to denote a sample.

3.34
sample extraction
act of extracting a portion (amount) of material from a larger quantity of material. This operation results in obtaining a sample representative of the batch with respect to the property or properties being investigated

Note 1 to entry The term can be used to cover either a unit of supply or a portion for analysis. The portion taken may consist of one or more sub-samples and the batch may be the population from which the sample is taken.

Note 2 to entry This operation is meant to obtain a sample representative of the material with respect to the property or properties being investigated.

Note 3 to entry The portion taken may consist of one or more sub-samples and the (sub-) samples may be the population sample representing the material.

Note 4 to entry This can be applied to a batch of materials produced (population from which the sample is taken).

3.35
sample holder
object which supports the specimen in the correct position for the sample preparation

EXAMPLE An example of sample holder is microtome holder.

3.36
sample inspection
analysis of the sample to determine information that is relevant for the subsequently applied characterisation method

EXAMPLE In the nanoindentation method, sample inspection is carried out by means of scanning electron microscopy to determine the indentation area.

3.37
sample preparation
sample preparation processes (for example, machining, polishing, cutting to size) are executed before actual observation and measurement

3.38
sample preparation parameter
settings of devices used for sample preparation

3.39
test case
characterisation experiment carried out to assess quality or performance against a defined reference or standard

3.40
user story
high-level description of the problem, including the material, the environment in which it functions and the properties/behaviour to be determined or explained

Note 1 to entry There are no details related to the characterisation process, which is to be decided on by the characterisation expert.

4 CHADA v2 introduction and guidelines

4.1 General

The CHADA provides modular templates to support a structured documentation of materials characterisation. Figure 1 shows a general representation of the CHADA documentation. For a more detailed representation of the characterisation workflow, please see Figure 2.

The CHADA consists of four sections:

a) user story;

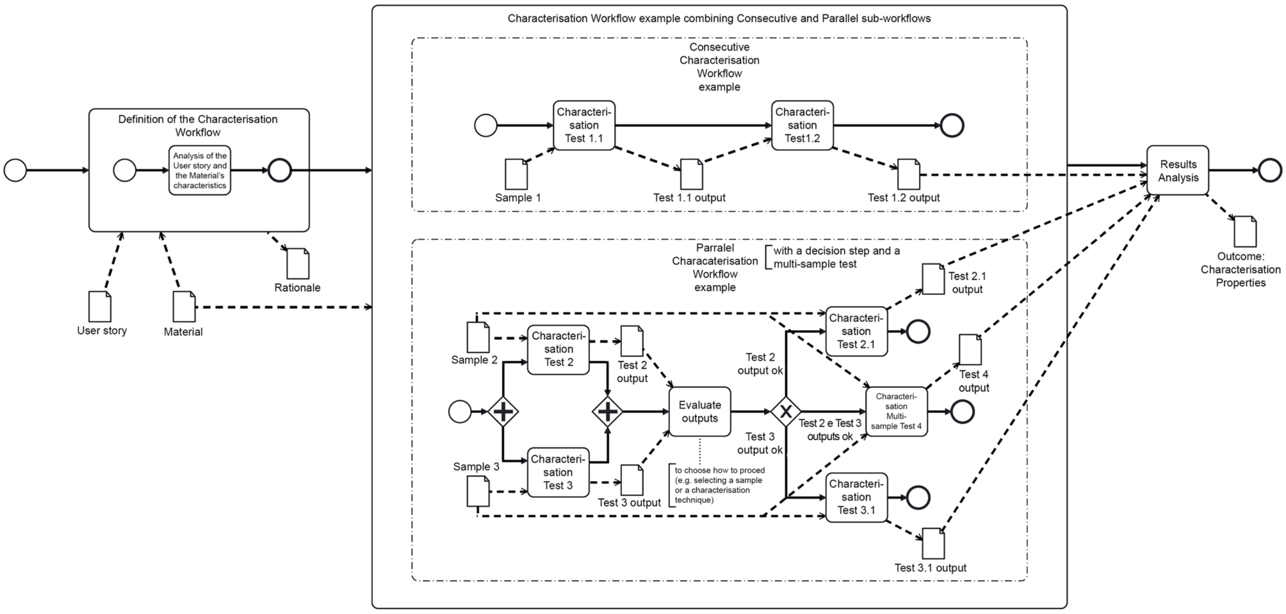
b) rationale;

c) characterisation workflow documentation including:

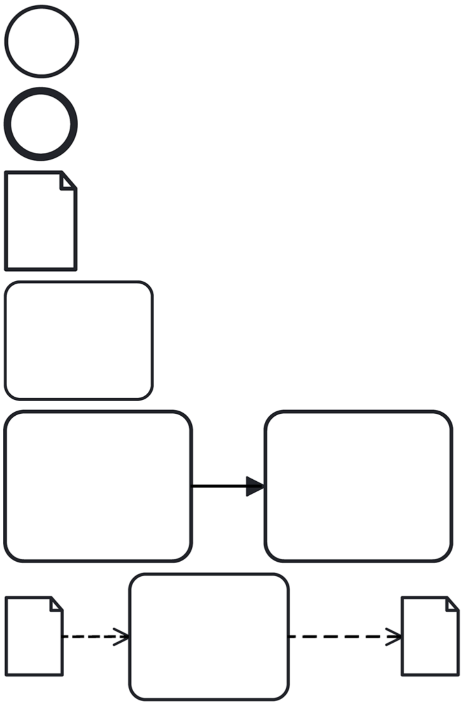
   1) diagram;

   2) workflow tables;

d) outcome.



Key



Start event

End event

Data object

Activity

Solid line: process flow

Dotted line: data flow (input, output of activities or processes)

Figure 1 — Graphical representation of the overall CHADA documentation, shown as a process in BPMN

With the CHADA, either a case of a single characterisation experiment/test case or sets of related characterisation experiments or test cases, carried out in response to a user story, can be documented. Any user can expand the CHADA with more detail when needed.

For diagrams in the CHADA, the BPMN 2.0 notation[5] should be used. BPMN is a standard set of diagramming conventions for describing business processes and has an XML serialisation format. It is designed

[5] Object Management Group Business Process Model and Notation, https://www.bpmn.org/

to visualize a rich set of process flow semantics within a process and the communication between independent processes.

Examples of using CHADA in different application cases are published on Zenodo, in the EMMC community[6].

4.2 User story

The user story documents the overall context, the question or issue to be addressed, and the desired information that the characterisation should provide. This can be the property of a material in a certain intended application-specific operational environment or the behaviour of a material during production.

4.3 Rationale

The rationale describes why the characterisation approach was chosen to address the user story. If possible, emphasise the choice by means of, for example, a peer reviewed paper, article or reference to an industry standard. The rationale informs the choices made in the characterisation workflow, including the material(s) sampling, and the measurements, measurement conditions and data processing. Hence the rationale can be understood as providing the basis for the characterisation experiments or test cases documented in the characterisation workflow tables.

4.4 Characterisation workflow overview

The characterisation workflow can consist of parallel and/or consecutive experiments. The characterisation workflow can also include decision trees.

Each characterisation experiment or test is a process which consists of a series of subprocesses and tasks. Each task is documented in the tables with an input and an output.

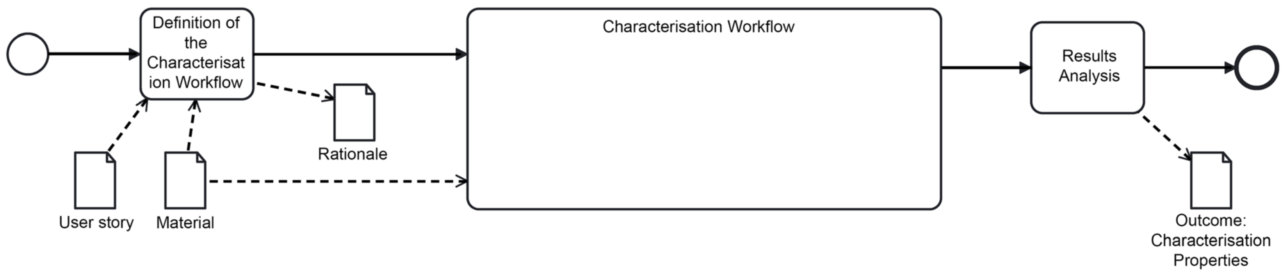
The documentation of the characterisation workflow starts with the description of the sample material, materials system, piece, volume to be tested.

Typically, a sample is extracted from the batch material. In non-destructive testing and in on-line monitoring, the volume to be tested is identified but not isolated.

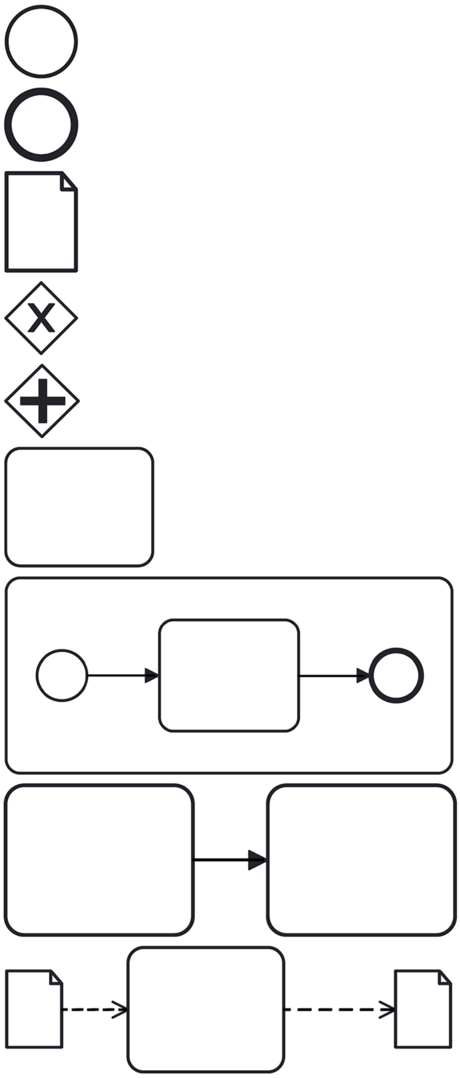
In each case, the sample is submitted to a measurement process using a device; the resulting raw data are then post-processed, leading to the output of the characterisation experiment.

The output of a characterisation experiment can be either qualitative, semi-quantitative or quantitative.

[6] Zenodo, EMMC ASBL – European Materials Modelling Council, https://zenodo.org/communities/emmc/



Key



Start event

End event

Data object

Exclusive gateway (decision point)

Parallel gateway

Activity

Sub-process expanded

Solid line: Process flow

Dotted line: Data flow (input, output of activities or processes)

Figure 2 — Graphical BPMN representation showing examples of consecutive and parallel characterisation workflows as well as decision trees. All notation follows the BPMN standard.

4.5 Diagram

A diagram of the characterisation workflow depicting the specific tasks, inputs and outputs documented in the workflow tables should be used. For diagrams in the CHADA, a standard graphical notation should be used, such as BPMN 2.0 (used in this document).

4.6 Workflow tables to document all experiments/test cases

For detailed documentation of all the experiments or test cases in a characterisation workflow, the CHADA section on characterisation experiment/test case modules (clause 5.4) provides templates for documenting all processes and related objects and data of the materials characterisation/test case. The entries can represent arrays, and multiple tables can be used to represent, for instance, a series of samples.

4.7 Characterisation outcome

The final CHADA section (clause 5.5) reports on the digested results of the characterisation workflow carried out. It can be understood as the response to the desired information described in the user story. If there is a series of test cases, then the answer to the user story is found by considering all results together.

5 CHADA v2 forms

5.1 CHADA section 1: user story

5.1.1 General

The user story is the question or issue that shall be addressed. In table 1, the high-level goal and/or need should be described, possibly without mentioning specific characterisation processes or techniques.

Table 1 — User story

User story	
Name	
Description	
Client/requester	

5.1.2 Material/materials system

Table 2 should describe the material/materials system of interest. It can be a single material, a multi-materials system or a component made of one or more materials.

Details about the specific material(s) or materials system and sample(s) characterised are specified in clause 5.4.

Table 2 — Material/materials system

Material/materials system	
Name	
Description	*(including any useful information about structure, composition, performance and properties)*
Reference to standard	*(add reference to standard/datasheet, if any)*
Further documentation	*(link to a relevant document/web resource)*

5.1.3 Environment and operating conditions

Table 3 should describe the environment and operating conditions in which the material or materials system is operating in its application, for example, pressure, temperature, humidity, or load.

Table 3 — Environment and operating conditions

Environment and operating conditions	
Description	
Further documentation	*(link to a relevant document/web resource)*

5.2 CHADA section 2: rationale

Table 4 should specify why the characterisation approach was chosen. If several tests are designed (for example, if several materials are going to be tested to find the optimal one, several loads are tested to find the breaking point) this can be documented by considering all concepts below to be arrays. The approach should be evidenced with a peer reviewed paper or article, if possible.

Table 4 — Rationale

Rationale	
Description	
Further documentation	*(link to a relevant document or resource)*

5.3 CHADA section 3: characterisation workflow overview

In Table 5, those who employ the CHADA should provide the metadata as well as a diagram to describe the overall characterisation workflow. The characterisation workflow can consist of parallel experiments or tests for different materials, different external loads or time series.

The laboratory, operator, and reference to standards can be specified here if they apply to the whole procedure. If applicable, they can be also indicated for each task separately in the respective tables.

Table 5 — Characterisation workflow metadata

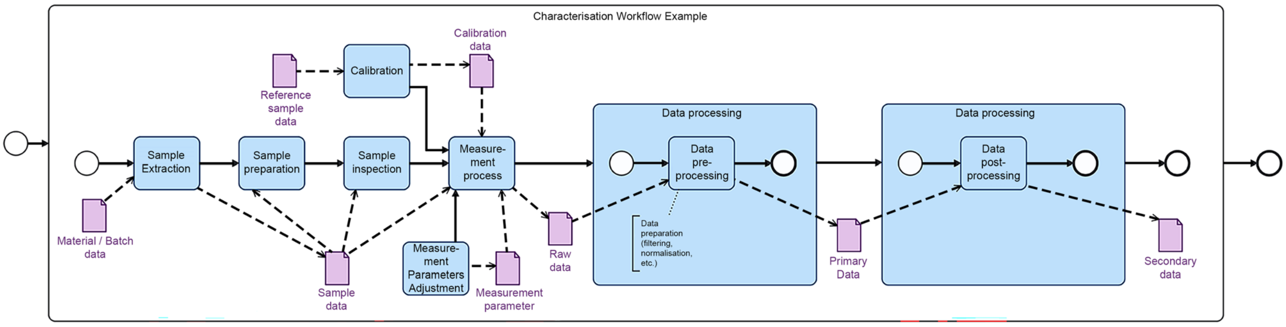
Characterisation workflow metadata	
Name	
Description	
Sample(s) to be tested	*(provide list of all samples)*
Test method(s) and environment(s)	*(all that are applied in the workflow)*
Reference to standard	*(add reference to standard, if any)*
Laboratory	
Operator	
Further documentation	*(link to a relevant document/web resource)*

Table 6 should provide a diagrammatic representation of the overall characterisation workflow from user story to outcome. A standard process modelling notation should be used.

Table 6 — Characterisation workflow diagram

Characterisation workflow diagram	
Put here a diagram (or diagrams) depicting all procedures (measuring and data processing) that constitute the overall characterisation case.	
Link to diagram	*(this may also lead to more detailed diagrams of different parts of the workflow.)*

For reference, a simple, generic characterisation workflow is shown in Figure 3. For each task (shown in blue), the CHADA contains a template documentation table. Data inputs and outputs are marked in magenta and correspond to particular rows in respective tables.

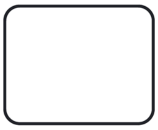


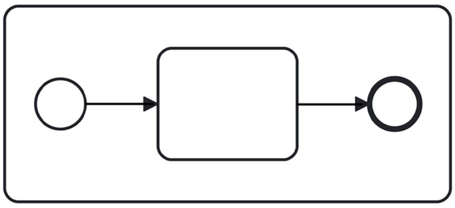
Key

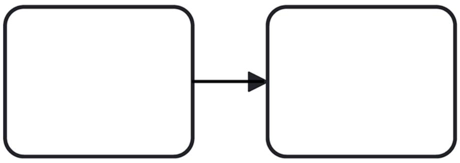

Start event


End event


Data object


Activity


Sub-process expanded


Solid line: Process flow

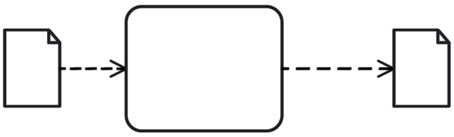

Dotted line: Data flow (input, output of activities or processes)

Figure 3 — BPMN diagram showing a generic characterisation workflow for one experiment or test

5.4 CHADA section 4: characterisation experiment/test case documentation

5.4.1 General

Each experiment and/or test procedure should be documented by using the following template tables. If several materials or samples are tested at one time or if a time series is measured, the measurements can be kept together by considering entities to be lists or arrays.

Time series measurements can be document by considering all boxes to be arrays. In this way, all measurements in a set can be documented together in one CHADA.

Table 7 and Table 8 document the material/materials system and sample(s) to be investigated in some detail. These have grey headers.

In Tables 9 to 16, and in the BPMN diagram, the characterisation workflow is documented, consisting of different processes (shown with blue headers) and datasets (magenta) as inputs and outputs. Here the material(s) and sample(s) are referenced just by data their unique identifier and/or unique name.

5.4.2 Material/materials system

In Table 7, the material, piece, volume, batch or materials system from which the sample/sample parts is extracted.

Table 7 — Material/materials system

Material/materials system	
Name	
Identifier(s)	*(for example, CAS number, batch identifier)*
Description	
Process history	*(including manufacturing steps or other prior processing information that describes the state of the material)*
Physical structure	*(if known prior to the characterisation)*
Composition / Chemical structure	*(if known prior to the characterisation)*
Properties known prior to the characterisation	

5.4.3 Sample

Table 8 has two fields to label the sample: name and identifier. The name is typically used in a human understandable way to uniquely label the sample status in different steps of the sample preparation, for example, raw sample, prepared (for example, polished) sample.

The identifier is typically an alphanumerical code that is used as a machine-readable way to identify and trace a sample throughout the steps of preparation and hence may be the same in different steps.

Table 8 — Sample

Sample	
Name	*(this can be a list of names denoting each step of sample preparation)*
Identifier	
Description	
Reference to standard	*(add reference to standard, if any)*
Further documentation	*(link to a relevant document/web resource)*

Dimensions	
Physical structure	
Material composition / chemical structure	
Other sample properties	
Hazard	*(link to a relevant document/web resource)*

5.4.4 Sample extraction

Table 9 — Sample extraction

Sample extraction		
Name (unique)		
Description		
Input: materials data	Material	
	Provider	
	Identifier	
	Description	
Laboratory		
Operator		
Instrument	Name	
	Manufacturer	
	Model	
	Unique ID	
Level of expertise of the operator and/or laboratory capabilities	*(with reference to relevant standards)*	
Level of automation	(*describe what can be automated in the process*)	
Reference to standard	*(add reference to standard, if any)*	
Further documentation	*(link to a relevant document/web resource)*	
Output: sample data	*(unique name or ID of sample, see also sample section for describing the sample in detail)*	

5.4.5 Sample preparation

In Table 10, the "instrument" information concerns the preparation of the sample.

Table 10 — Sample preparation

Sample preparation		
Name (unique)		
Description		
Input: sample data	*(unique name or ID of sample, see also sample section for a detailed description of the sample)*	
Input	*(from other steps of this characterisation procedure, other procedures or external data)*	
Laboratory		
Operator		
Instrument	Name	
	Manufacturer	
	Model	
	Unique ID	
Holder	*(in case the preparation involves mounting on a holder)*	
Parameters	*(settings for the preparation)*	
Environment	Description	
	Properties	
Level of expertise of the operator and/or laboratory capabilities	*(with reference to relevant standards)*	
Level of automation		
Reference to standard	*(add reference to standard, if any)*	
Further documentation	*(link to a relevant document/web resource)*	
Output: prepared sample data		

5.4.6 Sample inspection

Sample inspection is usually carried out through a characterisation technique. It is not meant to determine the investigated material's characterisation properties, rather to evaluate aspects that are relevant to the characterisation measurement (for example, the sample conditions and quality, the area of interest for the characterisation measurement).

Table 11 — Sample inspection

Sample inspection		
Name (unique)		
Description		
Input: sample data	*(unique name or id of the sample)*	
Input	*(from other steps of this characterisation procedure, other procedures or external data)*	
Laboratory		
Operator		
Instrument	Name	
	Manufacturer	
	Model	
	Unique ID	
Parameters	*(settings for the inspection)*	
Level of expertise of the operator and/or laboratory capabilities	*(with reference to relevant standards)*	
Level of automation		
Reference to standard	*(add reference to standard, if any)*	
Further documentation	*(link to a relevant document/web resource)*	
Output		

5.4.7 Calibration

Table 12 — Calibration

Calibration	
Name (unique)	
Description	
Input: reference sample data	*(specify in case of a reference sample, reference material or a certified reference material)*
Input	*(from other steps of this characterisation procedure, other procedures or external data)*
Laboratory	

Operator		
Instrument	Name	
	Manufacturer	
	Model	
	Unique ID	
Parameters (settings)		
Level of expertise of the operator and/or laboratory capabilities	*(with reference to relevant standards)*	
Level of automation		
Reference to standard	*(add reference to standard, if any)*	
Further documentation	*(link to a relevant document/web resource)*	
Output: calibration data		

5.4.8 Measurement parameters adjustment

Table 13 — Measurement parameters adjustment

Measurement parameters adjustment	
Name (unique)	
Description	
Input: sample data	*(unique name/id of the sample, see also sample section)*
Input	*(from other steps of this characterisation procedure, other procedures or external data)*
Laboratory	
Operator	
Level of expertise of the operator and/or laboratory capabilities	*(with reference to relevant standards)*
Level of automation	
Reference to standard	*(add reference to standard, if any)*
Further documentation	*(link to a relevant document/web resource)*
Output: adjusted settings for the instruments	

5.4.9 Measurement process

Table 14 — Measurement process

Measurement process		
Name (unique)		
Description		
Input: sample data	*(unique name/id of the sample, see also Sample section)*	
Input	*(from other steps of this characterisation procedure, other procedures or external data)*	
Laboratory		
Operator		
Level of expertise of the operator and/or laboratory capabilities	*(with reference to relevant standards)*	
Level of automation		
Reference to standard	*(add reference to standard, if any)*	
Further documentation	*(link to a relevant document/web resource)*	
Instrument	Name	
	Manufacturer	
	Model	
	Unique ID	
Parameters		
Probe		
Interaction volume		
Detector		
Environment	Description	
	Properties	
Characterisation signal		
Output: raw data		

5.4.10 Data processing

Table 15 should be used for all types of data processing, including data normalisation, data filtering, post-processing, measurement uncertainty calculation, calibration.

A series of Table 15 should be used for the respective data processing tasks specified in the "Type of data processing" entry.

Table 15 — Data processing

Data processing	
Name (unique)	
Description	
Input: <name> (raw data, primary data)	*(from other steps of this characterisation procedure, other procedures or external data)*
Type of data processing	*(for example, data normalisation, data filtering, post-processing, measurement uncertainty calculation)*
Data processing model	
Data processing software	
Laboratory	
Operator	
Level of expertise of the operator and/or laboratory capabilities	*(with reference to relevant standards)*
Level of automation	
Reference to standard	*(add reference to standard, if any)*
Further documentation	*(link to a relevant document/web resource)*
Output: <name> (primary data, secondary data)	

5.5 CHADA section 5: results analysis

Table 16 should be used to show the digestion of the output (post-processed data) of all relevant characterisation procedures to get to the material properties and/or behaviour that were requested in the user story in clause 5.1. It should include the interpretation and explanation of results.

Table 16 — Results analysis

Results analysis	
Input: the output of the above documented experiments or tests	
Method: description including method by which results were obtained across several characterisation procedures or test series	
Output: interpretation and explanation of final results, called outcome	
Further documentation	*(link to a relevant document/web resource)*

Bibliography

[1] Object Management Group Business Process Model and Notation. https://www.bpmn.org/

[2] Characterisation Methodology Domain Ontology (CHAMEO), https://github.com/emmo-repo/domain-characterisation-methodology

[3] IUPAC Compendium of Chemical Terminology. (https://goldbook.iupac.org/terms/view/S05661).

[4] Fair Go. https://www.go-fair.org/

[5] Guilbault G.G., Hjelm M. Nomenclature for automated and mechanised analysis (Recommendations 1989). *Pure Appl. Chem*. 1989, 61 (9) pp. 1657–1664 https://doi.org/10.1351/pac198961091657

[6] Nordberg M., Duffus J., Templeton D.M. Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003). *Pure Appl. Chem*. 2004, 76 (5) pp. 1033–1082 https://doi.org/10.1351/pac200476051033