# MACRAMÉ

# Provisions for the Inclusion of Safety Data in the Digital Materials Passports

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## Complex Relationships – the MACRAMÉ's R&I Approach

From monitoring of production of materials to their later life cycle stages, such as like end-of-life or possible circular re-integration, the value-chains of industrial materials are increasingly relying on **digital approaches**. The inclusion of safety data into the digital tracking of materials properties is not only a useful and sensible extra at this stage; rather, it is of utmost importance that the **complex relationships between the structure, functionality and safety of a material** are included into the data and design models that are being developed now to form the basis of the 'by design' character of fully digitalised materials value chains.

The MACRAMÉ Project has devised **an R&I approach, that widens the development** of harmonised test guidelines (TGs) and guidance documents (GDs) (OECD) and standards (CEN, ISO**) to market-relevant Advanced Materials (AdMas) in their complex product matrices** (Figure 1).

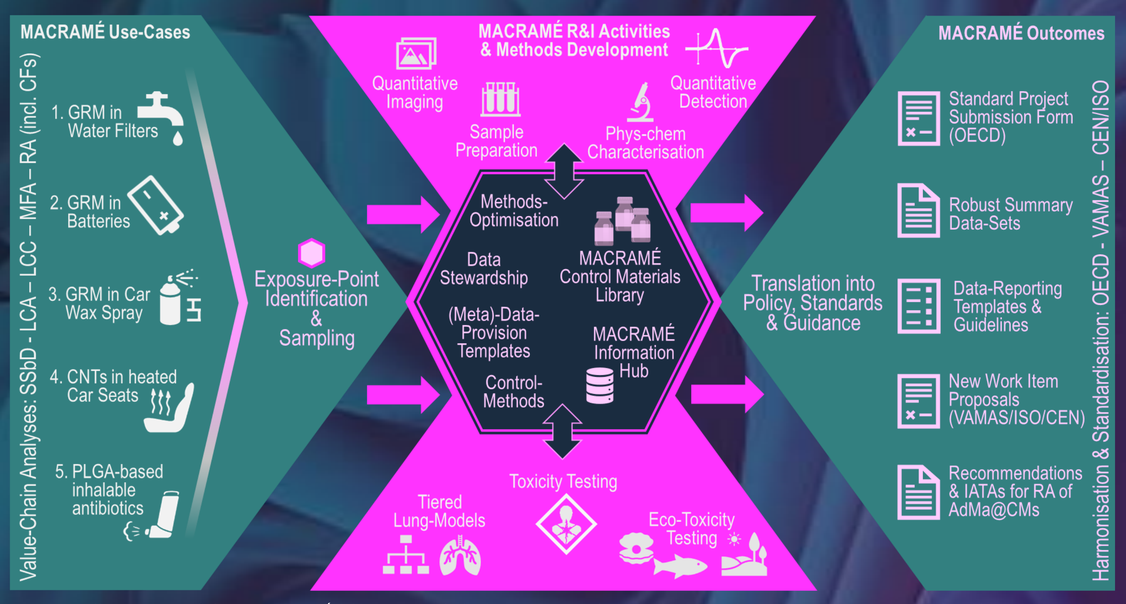


Figure 1: Illustration of the MACRAMÉ R&I Approach (AdMa@CMs: Advanced Materials in complex matrices; CF: Characterisation Factor; GRM: graphene-related material; IATA: integrated approaches to testing and assessment; LCA: Life-Cycle Assessment; LCC: Life-Cycle-Costing; MFA: Material-Flow Analysis; RA: Risk-Assessment; SSbD: Safe-&-Sustainable-by-Design).

This is achieved by defining the R&I Strategy through **life-cycle assessment of five market-relevant industrial MACRAMÉ Use-Cases** for the development of improved reporting guidelines combining community standards for materials characterisation and safety data with detailed descriptions of the complex product, biological and environmental matrices, based on the analyses of samples extracted at pre-identified MACRAMÉ Exposure-Points (Figure 2).

| MACRAMÉ Exposure Points [Samples & Constituents] | Pristine AdMa Manufacture | AdMa (Un-)Bagging & Transport | Product Manufacture | Reactor/ Machine Cleaning | (Un-)Bagging & Transport | (Professional) Intended Use | End-of-Life: Shredding | End-of-Life: Incineration | End-of-Life: Release/Leakage |
|---|---|---|---|---|---|---|---|---|---|
| | [AdMa] | | [AdMa] - [AdMa@CPM] - [CPM] | | | | [AdMa@EoL(CPM)] - [CPM(EoL)] | | |
| MACRAMÉ Use-Cases & Sample-Description @ Exposure Points: UC1: GO in Water-Filters | Pristine GO, polysulfone (matrix) | | GO@Polysulfone-Fibre, Water from the spinning-process | | | ~~(filtered water)~~ * | - | Incineration products: Fly-ash, Flue-gas | |
| UC2: FLG in BMS | Pristine FLG, epoxy resin | | FLG@epoxy (non-reticulated (liquid samples) and reticulated (solid samples))** | | | FLG@epoxy (overheated) | FLG@epoxy (shredded) | | |
| UC3: GRM-bearing Sprays | - | | | | | GRM@aerosol | GRM@aerosol (in container), EoL according to container material and/or special instructions | | |
| UC4: CNTs in Polymer Foils | Commercial CNTs (NanoCyl SA), polyurethane (PU) matrix | | CNTs@PU (masterbatch & cured composite) | | | CNTs@PU (overheated, abraded (Taber)) | CNTs@PU (shredded) | Incineration products ($O_2$-depletion): Fly-Ash, Flue-gas | |
| UC5: PLGA-based inhal. Antibiotics | PLGA-particles (different sizes) Ciprofloxacin | | ciprofloxacine@PLGA controls: Au@PGLA, $Fe_3O_4$@PLGA, PLGA (labelled with Lumogen red®) | | | | - | | ciprofloxacine@PLGA |
| Characterisation - Detection – Imaging (by Attributes) [Samples & Constituents] | All UCs: • characterisation; • aerosol generation & characterisation; • stability in environmental & biological matrices; • high resolution imaging in cells | | All UCs: • Aerosol generation for *in vitro* exposure • Characterisation of the generated aerosol • Stability and release in environmental & biological matrices | | | | All UCs: • EoL leaking from container/matrix • Aerosol generation for *in vitro* exposure • Stability and release in environmental & biological matrices | | |
| | | | UC1, UC2, UC4, UC5: • Identification, quantification & characterisation | UC1, UC2, UC4, UC5: • Identification of (form of) release during cleaning | UC3: • Identification: presence of GRM ➢YES: quantification, characterisation | UC2, UC4: • characterisation after mechanical abrasion (Taber) • characterisation of release at heating | UC1, UC2, UC4: • characterisation after mechanical abrasion | UC1, UC2, UC4: • characterisation of flue-gas & fly-ash | UC1, UC2, UC4: • Identification of release of EoL-products (in land-fill) |
| | [AdMa] - [AdMa@EM] - [ AdMa@BM] | | [AdMa@CPM] - [AdMa@CPM@EM] – [AdMa@CPM@BM] | | | | [AdMa@EoL(CPM)] – [AdMa@EoL(CPM)@EM] | | |
| Human Toxicity Testing (in-vivo – ex-vivo) [Samples & Constituents] | In case of inhalable release: Scheduled Tiered Lung-Model Approach (see Section 1.2, III.vii) | | | | | | | | |
| | [AdMa@BM] | | [AdMa@CPM] [AdMa@CPM@BM]- [AdM@BM] - [CPM@BM] | | | | | [AdMa@EoL(CPM) | |
| Ecotoxicity Testing [Samples & Constituents] | Ecotox Testing Strategy (see Figure 5) | | | | | | | | |
| | [AdMa@EM] | | [AdMa@EM] – [AdMa@CPM@EM] - [CPM@EM] | | | | [AdMa@EoL(CPM)] | [AdMa@EoL(CPM] | |

Figure 2: Schematic overview of the identified product-relevant MACRAMÉ Exposure-Points and the sampling, characterisation/imaging/detection and testing to be conducted at these points; *3 GRMs will be processed to a GRM reinforced epoxy composite according to Netkueakul et al. (2020).

In this course, the **MACRAMÉ Information Hub** has become the **one-stop sharing platform for all Project partners**; it ultimately aims to become directly integrated into advanced analysis, grouping and read-across applications, with the aim to strengthen European competitiveness.

## Interoperability – the MACRAMÉ Data Shepherd

To achieve full digital documentation (e.g. as part of a digital material passport) and data **interoperability** within MACRAMÉ, all (meta)data is mapped onto the harmonised data schema and transformed accordingly. To reduce the time for doing this, the data collector software library is being developed by the Project's **data shepherd** 7P9. This **library** is used to extract data from partner-specific data files, to automatically translate the data according to user-provided rules and to enrich the data by querying public services. After the assumed data producer has uploaded a data file shared project drive, the semi-automated workflow commences (Figure 3).

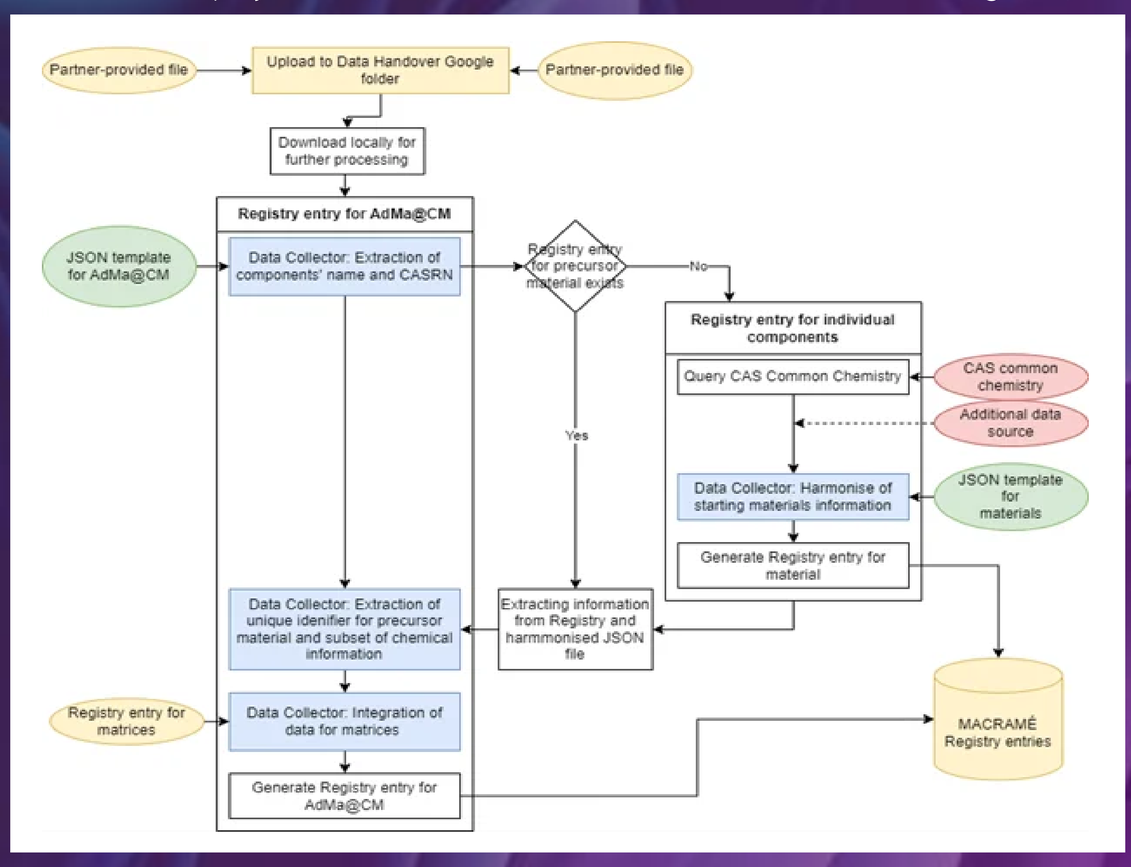


Figure 3: Schematic illustration of the workflow deployed to extract information on the AdMa from partner-provided files as well as public webservices.

## Knowledge Generation – the MACRAMÉ Processor

Complementing established, validated characterisation methods with the advanced MACRAMÉ methods as input for both **regulatory grouping**, **read-across** and **risk assessment** methods, as well as the for the scoping of **Safe and Sustainable by Design (SSbD)** initiatives, has the potential to increase the predictability and reliability of these methods. The new, advanced methods show the quality by providing information on the **robustness**, **reliability** and **validity** of the method in that they **come with highly increased information requirements** to be provided with each data point. This **data generation process** is depicted in Figure 4; it requires a very intense two-way exchange (of information and knowledge) between the WPs and is based on the development of new characterisation methods and their validation of them via the industrial Use-Cases.

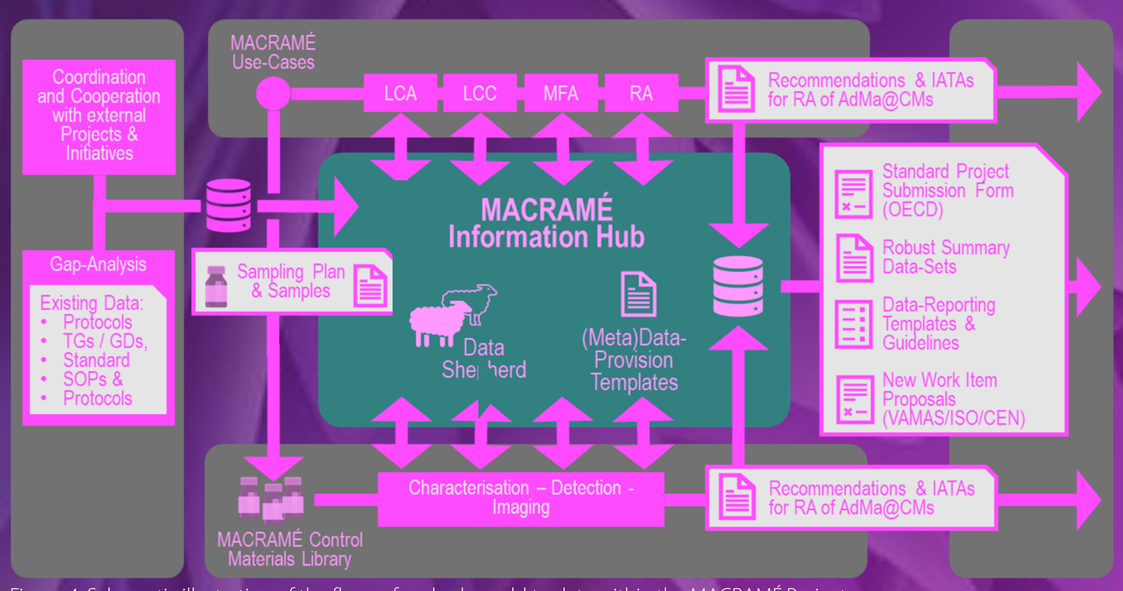


Figure 4: Schematic illustration of the flow- of and value-add to data within the MACRAMÉ Project.

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