Multidimensional Integrated Quantitative Approach To Assess Safety And Sustainability Of Nanomaterials In Real Case Life Cycle Scenarios Using Nanospecific Impact Categories

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1. Introduction

The INTEGRANO project addresses shortcomings and gaps in current safe and sustainability assessment approaches of Nano Materials (NMs) and Nano-enabled products (NEPs). Following the Framework for Safe and sustainable by design chemicals and materials[1], the project proposes a general assessment approach based on quantitative evidence to be applied in practice for specific Nano Materials (NMs) design cases.[2] The project will develop novel NMs impact categories (ICs) for nanotoxicity and eco-nano-toxicity assessment for the integrated application of standardised assessment methodologies. The synthesis, incorporation, use phase and end-of-life NMs life cycle stages (LCS) will be addressed for targeted case studies by leveraging the results and the results of case studies and methodology developed in the ASINA project[3-8], The collected/generated data will be used to meet the project's objectives to formulate design hypotheses and make design decisions by applying a data-driven approach and methodology, providing stakeholders with a digital supported decision process to tackle the Safe and Sustainable by Design (SSbD) challenge in the NMs context[9-11].

2. INTEGRANO – A general SSbD assessment approach based on quantitative evidence

INTEGRANO implements a defined protocol for the SSbD analysis of NMs and NEPs, relying on quantitative assessment supported by generation of a specific and harmonised dataset produced across a range of experimental and modelling activities (Figure 1) referred to a defined design of experiment matrix. The collection, storage and sharing of data within the INTEGRANO project will be mediated through the bespoke INTEGRANO Data Management Platform and associated INTEGRANO database. The Data Management Platform provides a structured interface to ensure that data

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collection across the life cycle stages is complete with respect to what is required to achieve the goals of the project and ensures that for each case study a harmonised dataset is produced which adheres to F.A.I.R. data principles. INTEGRANO proposes quantitative case-specific, and human-centric methodology, which is supported by the artificial intelligence algorithm also implemented within the ASINA project, enabling the selection of SSbD solutions by simultaneously addressing multiple and composite KPIs related to the safety, environmental, economic and functional dimensions. The methodology associates the generated harmonised data set to a specified DoE matrix. The advantage is found in the inherent minimum number of necessary and sufficient specific tox and eco-tox F.A.I.R. primary, functional and physicochemical data required, which implies minimising the experimental burden, while reducing the time and cost for developing each NM design case study. The SSbD cases represented in the decision spaces are associated to the corresponding performance level reported in the performance space and to the corresponding physicochemical SSbD cases data, thus enabling correlation between NMs physicochemical features and their related functional performance, safety and sustainability level. This opens up routes to further scientific investigations and grouping theory developments.

Overall, the SSbD workflow and related data generation and processing is organised in four stages:

i. Goal and scope definition.
ii. Data generation and Inventory by experimental and modelling work, data curation and F.A.I.R.ness compliance assessment.
iii. SSbD impact assessment: digital computation of the set of SSbD solutions with INTEGRANO Decision Support Tool.
iv. Interpretation of results, possible protocol reiteration, or final decision on the SSbD selected case operated by the NM (NEP) designer (decision maker).

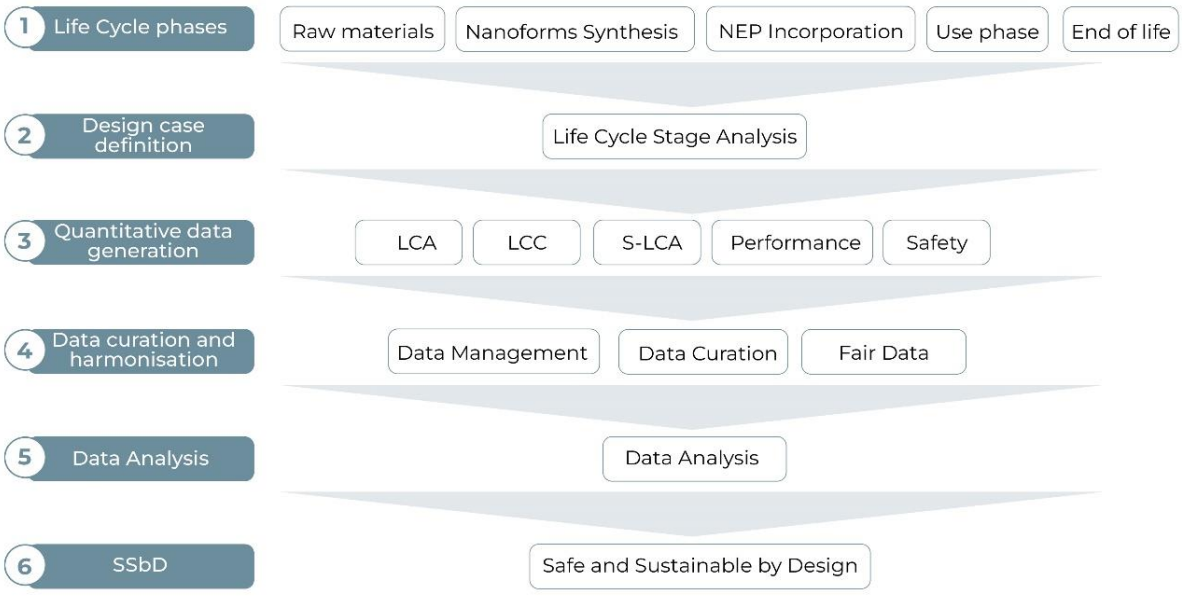

Figure 1 General view of data generation from each Life Cycle Phase towards the generation of the Safe and Sustainable by Design solutions by the INTEGRANO Decision Support Tool.

3. Conclusions

The methodology presented is a case-specific evidence based quantitative approach to SSbD within nanomaterials manufacturing, and which can be extensively applied more generally across materials and chemicals development. The approach requires a minimum amount of experimental data; thus, it is particularly suitable for research and development activities, also leading to enhanced feasibility for implementation in industrial production design cases where minimal prior data is available. By leveraging the artificial intelligence algorithm implemented in the MultiOpimal™ decision support system the proposed methodology allows for informed human-centric decision making in the development of nanomaterials and nano-enabled products. This translates into research and technological development cost and time reductions, with >95% reduction in time-to-market, opening new frontiers in science and material engineering as well as in synthesis of new chemicals based on a quantitative and predictive approach.

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5. References

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