Towards a nano-specific, quantitative based and human centric-SSbD Approach: Antibacterial nanocoatings case study

Massimo Perucca [1], Paride Mantecca[2], Benjamin Murray[1], Andrea Garrone[1], Mattia Costamagna[1], Anna Luisa Costa[3], Magda Blosi[3], Irini Furxhi[3], Rossella Bengalli[2], Juliana Oliveira[4], Franco Belosi[5], Alessia Nicosia[5], Jesus M. Lopez de Ipiña[6]

1. Introduction

The need of applying a Safe and sustainable by design (SSbD) strategy to the development of new chemicals and materials finds its main reference guidelines in the EU SSbD Framework[1]. For nano-forms and nano-materials diverse quantitative and semiquantitative SSbD implementation approaches have been investigated within the nano-materials community. However, industrial implementation of the SSbD approach within the engineered nanomaterials arena remains limited and requires support to maximise the advantages of the framework. Towards this, the ASINA[2-10] and INTEGRANO[11] projects aim to support the fast industrial uptake of nanotechnology by providing SSbD solutions and supporting tools.

2. A general SSbD assessment approach based on quantitative evidence

Here, a quantitative, case-specific, and human-centric methodology is proposed supported by the artificial intelligence algorithm implemented within the ASINA and INTEGRANO projects, enabling the selection of SSbD solutions by simultaneously addressing multiple and composite KPIs related to the safety, environmental, economic, and functional dimensions. The methodology requires generating a harmonised data set associated 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 data required, which implies minimising the experimental burden, while reducing the time and cost for developing each NM design case study. Indeed, a limited amount of experimental samples representing design alternatives needs to be generated, whose number depends on the number of key decision factors (KDFs) that are thought of affecting the addressed key performance indicators (KPIs).

[1] Project HUB360, Italy; massimo.perucca@project-sas.com, benjamin.murray@projecthub360.com
[2]University of Milano-Bicocca, Italy; paride.mantecca@unimib.it
[3]Consiglio Nazionale delle Ricerche - ISSMC, Italy
[4]CeNTI - Centre for Nanotechnology and Smart Materials, Portugal
[5]CNR-ISAC, 40129 Bologna, Italy
[6]TECNALIA, BRTA, Miñano, Spain

3. Case study – antibacterial nano-coatings

Case studies for the development of antibacterial nano-coatings investigated within the ASINA project through the ASINA-ES decision support system are presented addressing the NMs synthesis and incorporation life cycle stages. The need to integrate the environmental and safety assessments through the development of nano-specific eco-toxicity and human-toxicity indicators addressed in the INTEGRANO project will be presented as an enabling approach for the exploitation of existing international standardised assessment methodologies with defined protocols and metrics such as ISO1040-44 for Life cycle assessment.

Figure 1b: By selecting one point in performance space, ASINA-ES returns the corresponding point in the decision space (blue circled cross), by specifying the values of synthesis Key Decision Factors (KDFs).

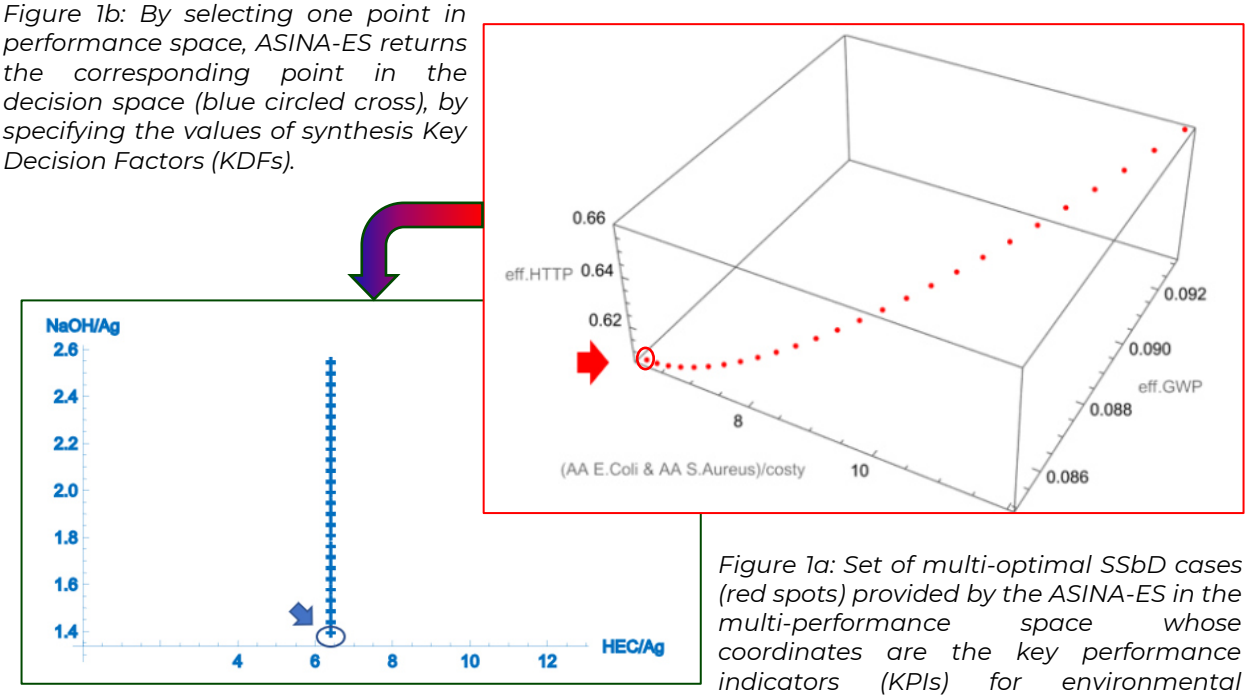

Figure 1a: Set of multi-optimal SSbD cases (red spots) provided by the ASINA-ES in the multi-performance space whose coordinates are the key performance indicators (KPIs) for environmental sustainability (GWP), Human toxicity (HTTP) and composite antibacterial functionality-cost KPI.

4. Conclusions

The methodology presented is a case-specific evidence-based quantitative-approach to SSbD within nanomaterials manufacturing, and which can be extensively applied across materials and chemical development. This approach requires production of a restricted set of experimental samples and generation of a minimum and sufficient number of harmonised related data, leading to enhanced feasibility for implementation in industrial research and development of design cases where minimal prior data is available. This translates into research and technological development cost and time reductions, with >95% reduction in time-to-market. The proposed SSbD methodology corroborated by the MultiOptimal™ decision support system based on artificial intelligence algorithms offers the product designer and decision makers with a refined set of SSbD options on which informed human-centric decisions may be taken within the framework of SSbD nanomaterials and nano-enabled products development. The application of the methodology and the use of MultiOptimal™ for the specific design case study addressed to the development of antibacterial nano-coatings, allowed material designers from CNR to identify the best SSbD synthesis option starting from six

representative design options. Indeed, the selected protocol for the synthesis of the organic-inorganic nano-silver product complies with the lowest environmental impact and the least human toxicity level attainable within the design space defined by the two synthesis key decision factors (NaOH/Ag and HEC/Ag ratios), while the obtained product offers the maximum functionality attainable among the different design options.

5. Acknowledgements

The two-step development of this work has been possible thanks to the ASINA and INTEGRANO projects, ASINA received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862444; INTEGRANO received funding from the European Union's Horizon Europe research and innovation programme under GA No 101138414.

6. References

1. Caldeira, C. et. al (2022) Safe and sustainable by design chemicals and materials - Framework for the definition of criteria and evaluation procedure for chemicals and materials, ISBN 978-92-76-53264-4, doi:10.2760/487955, JRC128591.
2. Perucca, M, A multicriteria decision tool to address Safe-by-Design solutions for nanomaterials and nano-enabled products, NanoTox2021, 10th International Conference on Nanotoxicology, book of abstracts, p245.
3. Furxhi L et. al (2022) ASINA Project: Towards a Methodological Data-Driven Sustainable and Safe-by-Design Approach for the Development of Nanomaterials. Front. Bioeng. Biotechnol. 9:805096. doi: 10.3389/fbioe.2021.805096.
4. Faccani, L et. al (2022) Multi - criteria optimization approach applied to photocatalytic nano-structured systems for waste-water remediation, Nano-Week and NanoCommons Final Conference, June 20-24, Cyprus. (oral presentation).
5. Perucca, M. (2022) ASINA-ES: a decision support system for Safe ad Sustainable By Design to simultaneously comply with: costs, sustainability, environment and safety, methods, tools, and technologies for ssbd purposes Nano-Week and NanoCommons Final Conference, June 20-24, Cyprus. (oral presentation).
6. Perucca, M. (2023) ASINA project exploitation workshop: SSbD industrial application in cosmetics, textile and other sectors, ASINA-Expert System, Nano Innovation 2023, Rome.
7. Perucca M. et. al (2023), ASINA-ES: A Quantitative Based Decision Support Tool for Multi-Optimal Safe and Sustainable by Design Solutions, Methods, Tools, & Technologies for SSbD Purposes, NanoSafe 2023.
8. Blosi M. et. al (2023) Design strategies supporting the development of antiviral nano-Ag-based materials under a ssbd approach, NanoSafe2023.
9. Brigliadori A. et. al (2023) Implementation of Design Strategies to Reach the Desired SSbD Performance Attributes: Functional Textile Coatings Case Study, Nanotox 2023.
10. Perucca M., Costamagna M., (2023) ASINA cosmetic NEPs case study: scaling up for the Step 4, European Commission 4th Stakeholder workshop on "Safe and sustainable by design", 6th December 2023, Brussels.
11. Perucca M., (2024) An integrated quantitative approach in Safe and Sustainable by Design decision support systems: from ASINA to INTEGRANO Expert Systems, - Safe-by-design tools and technologies for nanomaterials, ANTHOS 2024, 5 March 2024, Vienna.