

Safe-and-Sustainable-by-Design for Advanced Materials - A case study on the agricultural use of imogolites

Veronique Adam¹, Fabienne Testard², Dorra Gargouri², Arianna Filoramo², Susan Dekkers³, Veronica di Battista^{4,5}, Wendel Wohlleben⁵, Blanca Suarez-Merino¹

1. Introduction

Following the European Commission Recommendation for a European assessment framework for 'safe and sustainable by Design' (SSbD) chemicals and materials (European Commission 2022), the HARMLESS project built a SSbD framework tailored to Advanced Materials (AdMa). Based on this framework, an online Decision Support System, directed towards innovators, is being created.

2. Materials and method

In this study, functionalised imogolites developed for agricultural purposes (imogolite_OH, imogolite_CH₃, Cu-doped imogolite_CH₃) are taken through a flexible stage-gate innovation process and used to test the HARMLESS framework and decision support system. At the ideation and business case stage, the HARMLESS WASP module, composed of 14 questions to the user, raises potential concerns on safety and sustainability aspects of the different imogolites versions. At the second innovation stage (i.e. lab phase), key physchem, exposure, hazard and sustainability descriptors are measured to further define potential issues on the aspects that raised red flags.

3. Results

Differences among imogolite versions mainly come from increasing the complexity in terms of multi-component composition. Hazards could arise from components issued from the pristine materials such as gibbsite, alumina, silica, methyltrihydroxysilane and copper. Nevertheless, these AdMa show benefits towards sustainability as compared to benchmark materials (such as Cu salts), as they require less use of Cu. The contribution to several Sustainable Development Goals (SDGs) as defined by the United Nations, such

¹ TEMAS Solutions GmbH, Laetteweg 5, 5212 Hausen AG, Switzerland; veronique@temasol.ch

² CEA, Université Paris-Saclay, CNRS, NIMBE_ UMR 3685, LIONS, 91191 Gif-Sur-Yvette, France

³ TNO, Unit Health Living, Risk Analysis of Products in Development, Princetonlaan 6, 3584 CB Utrecht, the Netherlands

⁴ Technical University of Denmark, Department of Environmental and Resource Engineering, Building 115, Kgs. Lyngby, Denmark

⁵ BASF SE, Departments of Analytical and Material Science and of Experimental Toxicology and Ecology, Ludwigshafen, Germany

as sustainable food production (SDG 2), efficient use of resources (SDG 12) or clean water and sanitation (SDG 6) will be discussed regarding their composition and potential functionalities.

4. Outlook

The quantitative SSbD assessment currently taking place at lab phase on physchem characteristics (e.g. size, composition, dissolution rate), toxicity (e.g. inflammation potential, cytotoxicity) and sustainability descriptors (e.g. use of critical raw materials, release of hazardous chemicals) feeds the discussion on the balance between risks, benefits, costs and performance of each imogolite version and helps the selection of the most appropriate version to take to pilot phase.

5. References

European Commission (2022) Commission Recommendation of 8.12.2022 establishing a European framework for 'safe and sustainable by design' chemicals and materials. 7 pp.