Normalised similarity assessment to inform grouping of advanced multi-component nanomaterials by means of an Asymmetric Sigmoid function

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1. Introduction

Due to the increasing use of advanced multi-component nanomaterials (MCNMs) in various industries, there's a growing need to increase the efficiency of their safety testing while reducing the use of experimental animals. In this context it is relevant to adopt similarity-based grouping approaches as a basis for read-across of existing data for both safe by design and risk assessment purposes.

This document proposes a novel similarity assessment methodology specifically designed for MCNMs. This method groups similar MCNMs, allowing researchers to read-across safety information from well-studied materials to new ones. This reduces the need for extensive testing and animal experiments.

The methodology is implemented in a user-friendly software script and web application accessible to industry users, especially from small and medium-sized enterprises (SMEs). The document also presents a real-world example from the construction sector to demonstrate the added value of the proposed methodology.

2. Methods

A new method for assessing similarities between nanoforms is presented, particularly suited to the more complex identity of the advanced MCNMs. The method considers all available information on the materials' physical and chemical properties, as well as their toxicity. It incorporates a special scaling technique to ensure consistent comparisons across different properties.

This method allows for comparing MCNMs to each other, to groups of MCNMs, or even to single-component nanomaterials. The approach involves several steps: i) transforming data for consistency by application of the Arsinh function (i.e., Inverse hyperbolic sine); ii) scaling of properties to make them comparable by applying asymmetrical Logistic scaling function for scalar properties and full curve shape comparison by application of a modified Kolmogorov–Smirnov metric for bivariate properties; and iii) calculating similarities for each property, and then combining these

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to get an overall similarity score by the use of Ordered Weighted Average (OWA). To make it easier to use, the authors created a software script that automates these steps which was delivered as a web application.

3. Conclusions

A new way to compare properties of materials is introduced which is especially tailored to safety (toxicity). This method uses a special S-shaped curve (sigmoid function) to transform data into a format that's easier to compare and combine. This new approach ensures that comparisons remain consistent even when adding new materials for evaluation.

The authors tested their method on a real-world example from the construction sector: SiO_2-ZnO nanocomposite composed of SiO_2 core coated by ZnO. This material is used to ensure photocatalytic decontamination (NO_X gases removal) of construction materials such as mortar.

The results of applying the proposed method in the case study has demonstrates its effectiveness to identify similarities between multicomponent nanoforms, making it a valuable tool to support grouping as basis for safety assessment. The approach was helpful to point out that using different dispersion media has a propound effect on dissolution-related similarity. Although distance matrices for dissolution in different media are quite distinct, they all show a high dissimilarity for ZnO. Additionally, while the Zeta potential values are all similar, Size shows higher distances for ZnO too. The overall aggregated similarity further confirms these differences by displaying high dissimilarity for ZnO.

4. References

Zabeo, A., Basei, G., Tsiliki, G., Peijnenburg, W., & Hristozov, D. (2022). Ordered weighted average based grouping of nanomaterials with Arsinh and dose response similarity models. *NanoImpact*, *25*. https://doi.org/10.1016/j.impact.2021.100370