

REVIEW OF THE EXISTING TOOLS FOR THE OPERATIONALIZATION OF THE SAFE AND SUSTAINABLE BY DESIGN FRAMEWORK

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ABSTRACT

The European Union (EU), through the Chemicals Strategy for Sustainability (CSS)^[1] and the Zero Pollution Action Plan^[2], underlined the need for a climate-neutral and toxic-free environment and economy, emphasizing the shift towards a Safe and Sustainable by Design (SSbD) approach. The SSbD concept is a holistic approach seeking to integrate the safety and sustainability of chemicals and materials early in their design stage, considering the entire life cycle. The SSbD framework set by EC JRC^[3,4] encompasses five steps that assess both the safety and sustainability aspects of a chemical/material and is linked to the innovation process through the stage gate model^[5]. Within this context, we have conducted a comprehensive review of existing tools (models, software, methods) that hold the potential to serve the scope of SSbD. A thorough literature search was carried out with a primary focus on identifying tools that can facilitate safety and sustainability assessments for chemicals. The screening of the tools was based on specific key criteria such as their accessibility, the availability of comprehensive documentation, and their alignment with the requirements of the SSbD framework. In more detail, we categorized the tools into safety and sustainability assessment tools according to their estimates. Several types of tools have been identified, including quantitative structure-activity relationship (QSARs) (e.g. VEGA), exposure (e.g. INTEGRA), and life cycle assessment (LCA) models (e.g. USEtox). Based on our findings, the applicability domain of the identified tools mostly falls under the fields of exposure (occupational, consumer, and environmental) and environmental sustainability assessment, whereas there is a lack of tools in the socioeconomic assessment part. In terms of innovation, it is observed that QSAR models are prevalent at the earlier stages of innovation, while most of the tools can be applied at the later stages of innovation as data availability increases. We conclude that there are available tools that could facilitate to some extent the operationalization of SSbD. However, given the high complexity of SSbD, there is a need for integrative models and methodologies, such as New Approach Methodologies (NAMs) and Artificial Intelligence (AI) techniques, that could further enhance the current modelling framework.

KEYWORDS: Safe and Sustainable by Design, Models, Risk Assessment, Sustainability Assessment

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