Summary

The doctoral thesis explores the integration of Life Cycle Assessment (LCA) methodologies into the Safe and Sustainable by Design (SSbD) framework, focusing on the chemical sector. As SSbD aims at guiding innovation in chemical industry, robust and adaptable sustainability assessment tools become essential. The thesis addresses methodological challenges through four core chapters, each contributing to the practical application and advancement of LCA in SSbD contexts.

Chapter 1 presents the application of the SSbD framework to a case study involving six PVC plasticisers used in food contact materials. The author contributed to the environmental sustainability assessment using the Product Environmental Footprint (PEF) method within an LCA framework. The study highlights limitations in data availability and methodological challenges when applying LCA to the SSbD framework.

Chapter 2 investigates the issue of comparability in LCA for chemical products. By analysing the role of chemical nomenclature, intermediate classification, and dataset structuring, the chapter identifies the need for harmonised descriptors and system boundaries to enable meaningful comparison across substances. These findings are crucial for supporting alternative assessment within the SSbD framework.

Chapter 3 introduces a methodology to construct proxy processes for chemicals lacking detailed life cycle inventory (LCI) data. The tool maps synthetic pathways based on mass balances, allowing practitioners to trace back a substance's supply chain and build representative proxies. This method facilitates screening-level assessments for data-scarce or emerging substances, a frequent need in SSbD evaluations.

Chapter 4 applies an advanced LCA modelling approach to assess the environmental impact of European plastic consumption under different trade and energy mix scenarios. By incorporating import data and future-oriented energy transitions, the study adapts Ecoinvent datasets to reflect changes in electricity and heat generation both geographically and temporally. This work supports prospective assessments aligned with EU policy goals and sustainability transitions.

The thesis overall contributes to the enhancement of LCA as a flexible, forward-looking tool for SSbD. It addresses the limitations of existing datasets and methods, offering practical solutions through data adaptation, proxy creation, and scenario modelling. These contributions are directly applicable to policy development, sustainability screening, and innovation processes in the chemical and material sectors.