Challenges in Predictive Sustainability Assessment of Novel Lubricants following SSbD Principles

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1. Introduction

The global imperative to reduce carbon emissions has emphasized the importance of enhanced friction and wear management in tribological applications, potentially mitigating approximately 1460 Mt CO2 and 8.7% of the total energy consumption annually.[1] In low-carbon footprint sectors such as e-mobility and renewable energies, lubricants, play a central role in machinery requiring high durability, efficiency, and tribological performance. Despite their positive impact on reducing friction and wear, the intricate and often environmentally unfriendly composition of lubricants hinders their overall ecological benefits. Stringent regulations (and ecolabels), targeting specific chemicals (lithium-based additives, perfluorinated polymers, chlorinated paraffins), have been implemented by international authorities to address this challenge and are driving trends in the lubricant market. Nevertheless, while staying within the constraints of planetary boundaries, the thresholds for chemical novelties have been already surpassed [2]. Consequently, it is imperative that any novel lubricant is intrinsically non-toxic and environmentally sustainable. A guideline to comply with such criteria has been provided by the European Commission [3], the Safe-and-Sustainable by Design (SSbD) framework. However, with respect to initial testing of said framework in case studies [4], it was found that the framework possesses rather complicated and cost intense approach for the innovation process for already existing products.

2. Challenge and Approach

The challenge at hand involves to develop novel lubricants that comply with the SSbD framework but yet provide competitive function in their respective use cases. The SiToLub Horizon project aims to mitigate risks associated with non-toxic chemical introduction by establishing an integrated multi-functional and cost-effective **simulation environment** in respect to the SSbD framework. Within this environment, we are developing a predictive sustainability assessment tool focusing on all three dimension of sustainability.

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The uniqueness of the SiToLub project lies within its interdisciplinary approach to comply with SSbD criteria via simulation tools as well as to foresee the sustainability (Figure 1). To address these challenges comprehensively, we develop a Life Cycle Sustainability Assessment (LCSA) methodology tailored specifically for lubricants and their components. This methodology encompasses the entire lifecycle of lubricants, focusing in particular on use and end-of-life stages. By uniquely incorporating results from toxicity and performance simulation tools, we will capture the environmental performance and impact of lubricant systems comprehensively using our openLCA software platform. The combination with background databases (ecoinvent and PSILCA), allows us to perform the calculation of ecological, cost, and social LCA indicators already in the early product design stage.

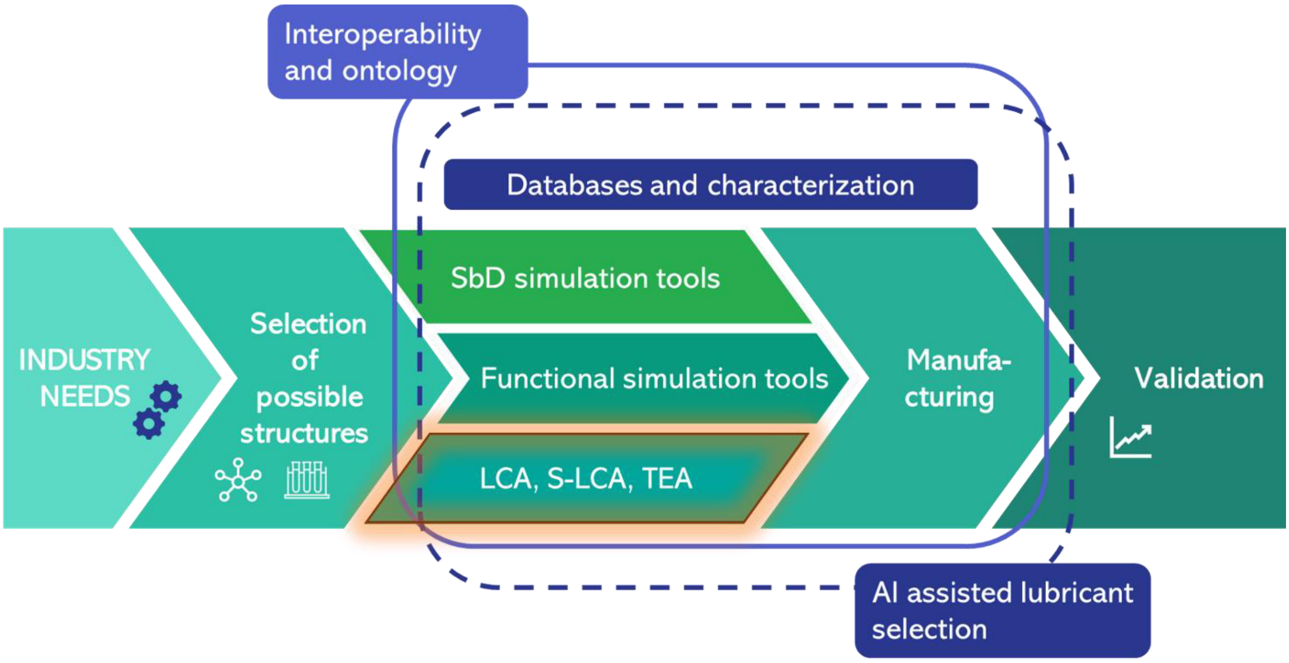

Figure 1: Work flow of SiToLub with focus on the sustainability assessment (ecologic, social and economic).

Although, the SSbD framework [3] focuses mostly on environmental and human health issues, the social impacts have been merely integrated into the assessment as displayed in case studies [4]. In combination with our PSILCA database [5] and system dynamics, we are simulating social impacts for the lubricant fabricant, usage and end of life using quantitative social LCA approaches.

The simulation approaches provided is the project will be finally validated by the production of SSbD-lubricants by industrial partners. (Figure 1). This will allow us to feedback our system dynamics and LCSA models improving the utilized simulation approaches.

3. Initial Results

The initial phase of our research has focused on laying the groundwork for developing a comprehensive LCA methodology for lubricants and integrating results of QSAR and performance modelling into our LCA models. Thereby, we have conducted an extensive review of existing literature, standards, and methodologies, synthesizing insights from diverse sources to inform our approach. For now, connecting QSAR results for (eco)toxicity and biodegradability, with the openLCA software, will require intensive mapping using the UseTox methodology. Yet, the translation of various toxicity values to LCA relevant data remains a challenge. Though, such an approach is eminent as we focus in particular environmental and health effects of lubricants during their use phase. Nevertheless, the outcome of such an harmonisation will provide a large impact on the SSbD-related simulation approaches.

Looking ahead, our research will focus on refining and validating our LCA methodology through case studies and empirical data collection. By integrating insights from ongoing projects and leveraging advances in computational modeling and data analytics, we aim to develop a robust framework for evaluating the sustainability performance of lubricants throughout their lifecycle. Ultimately, our goal is to provide stakeholders with actionable insights to inform decision-making and drive innovation in the development of energy-efficient and environmentally sustainable lubricant solutions.

4. Conclusions

The results of the SiToLub project serve as indicators for a simulation-based Safe-and-Sustainable by Design (SSbD) approach applicable to specialty chemicals across diverse industries. Additionally, this approach provides important and comprehensive insights into evaluating the sustainability of new materials in the early stages of the design process.

5. References

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