SiToLub - Simulation Tools for the design of safe and sustainable Lubricants

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1. Introduction

The need to promote a low carbon economy while ensuring effective actions to overcome the obstacles that the lubricant companies are facing (e.g. ever-changing regulatory restrictions on the chemicals, more demanding technical requirement of the industry, etc.) has led to the need for using computational models to accelerate the time to market of novel lubricant formulations. So far, each modelling case has been focused on understanding properties under specific conditions. The SiToLub project, funded under the HORIZON-CL4-2023-RESILIENCE-01 topic, aims at creating an integrated multi-functional digital simulation environment, supported by artificial intelligence, to help the lubricant manufacturers to face these challenges and move towards Safe-and-Sustainable-by-design (SSbD) materials and products by pre-assessing lubricant formulations at the design phase. SiToLub will integrate tools to predict human and environmental toxicity, to simulate properties and the interactions within the application environment, to estimate life-time product performance and efficiency during use phase, and to foresee the sustainability aspects of the new formulation.

2. Objective and methodology

SiToLub project aims to develop a digital tool/platform based on integrated computational models with built-in artificial intelligence (AI) features for the Safe and Sustainable by Design formulation of new lubricants. The tools developed will provide assessment of the safety (toxicity to humans, ecotoxicity to environment and workers risk) and, at the same time, sustainability guidance to design ecofluids (coolants, greases, oils) in a clear and holistic way regarding the foreseeable physico-chemical properties and tribological performance.

The safety assessment will be realized by using molecular dynamic models developed by the partners.

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The tribological models will allow the prediction of the energy consumption during use by providing friction force values and expected durability of the materials by using wear data about the materials in contact with different fluids. They will also provide information about the degradation of the fluids in use and the chemical reactions occurring. The models will be flexible enough to predict the behaviour of the materials for different working parameters applied for different applications (wind turbines, electric cars, industrial machining, etc.)

This ambitious and forward-thinking system will leverage on a series of tools, ranging from technical evaluation and prediction models (computational models supported by artificial intelligence), combined with established Life-Cycle Analysis (LCA) methodologies to consider the environmental, social and economic impact.

Interoperability must be ensured between experimental and modelling domains and between different knowledge domains to ensure an effective exchange of data and interaction. Harmonizing taxonomies, classifications, and definitions as well as documentation is essential for a seamless exchange of data and efficient liaison of different disciplines, their models, experimental techniques, and approaches. To systematize interoperability, a domain ontology will be created based on the top-level ontology EMMO [1], as well as other ontologies related to standardization of data documentation across different domains, as for example to materials and manufacturing.

To deal with data scarcity and insufficient data diversity, data augmentation and data synthesis methods will be applied to enable the simulation model to produce even more accurate results.

3. Outcome and exploitation

The final result of SiToLub will be an organic infrastructure composed by many interconnected elements, as represented in Figure 1.

The core of this infrastructure is the SiToLub platform that will store the data produced during and after the project and will harmonize them with the data coming from other existing databases, including the database of i-Tribomat and data directly produced by the SiToLub partners.

Another important section of SiToLub infrastructure is composed by the different computational models that will be developed during the project. As previously mentioned, 3 categories of models will be developed according to their purpose. The first category will be related to the assessment of toxicity and biodegradability of the components of the lubricants, to be sure that the formulation will be safe for the people and the environment. The second category of models is related to the prediction of the technical properties of the lubricants and their overall functionality. The last category of models will be used to assess the life cycle of the lubricants, and their impact on the society and on the economy.

Existing databases will be used to feed the modelling tools, but the reliability of the data used will be assessed by realizing experimental tests according to international standards or specifically developed protocols.

Anyway, the testing procedures for the assessment of safe and sustainable lubricants will be elaborated and will be an essential part of the SiToLub foundation.

Artificial intelligence methods will be used for producing synthetic data when needed and to select the best candidates as lubricant components.

To ensure sustainable industrial use of the project results, SiToLub project relies on the presence of the Open Innovation Test Bed i-Tribomat, that will be the core exploitation partner. The newly developed simulation methods, and the updated infrastructure previously described, will expand the services offered. Thus, European industry will have access, in addition to the materials characterization and simulation tools already developed, also to the newly built infrastructure for the SSbD formulation of lubricants.

Each of the simulation tools could be used as service for the evaluation of the properties and performance of the lubricants and their additives.

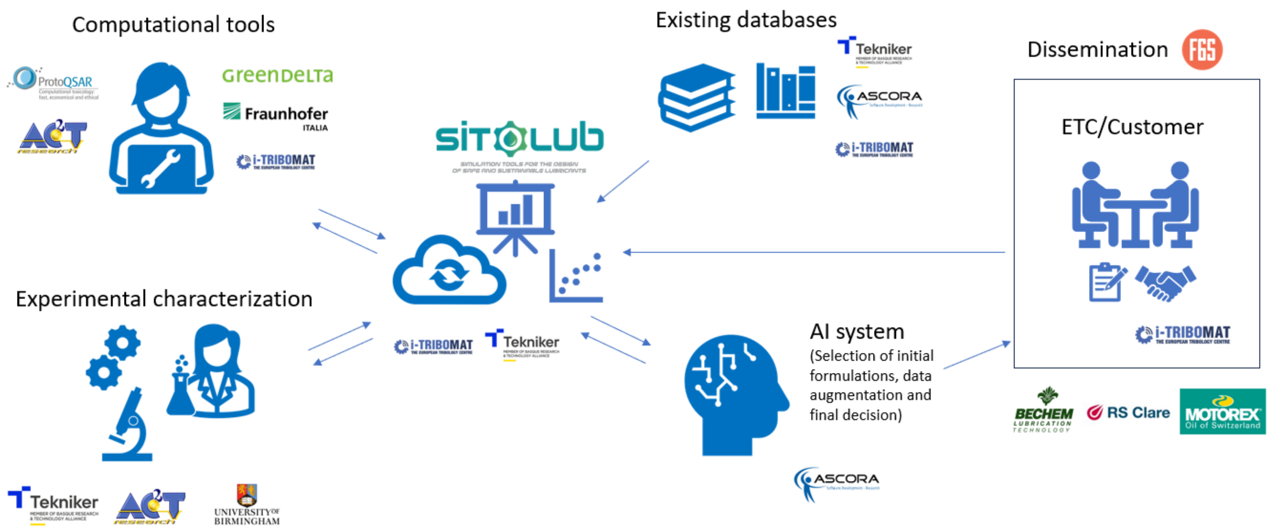

Figure 1. Exploitation structure of SiToLub

4. References

[1] Elementary Multiperspective Material Ontology (EMMO).
https://emmo-repo.github.io/