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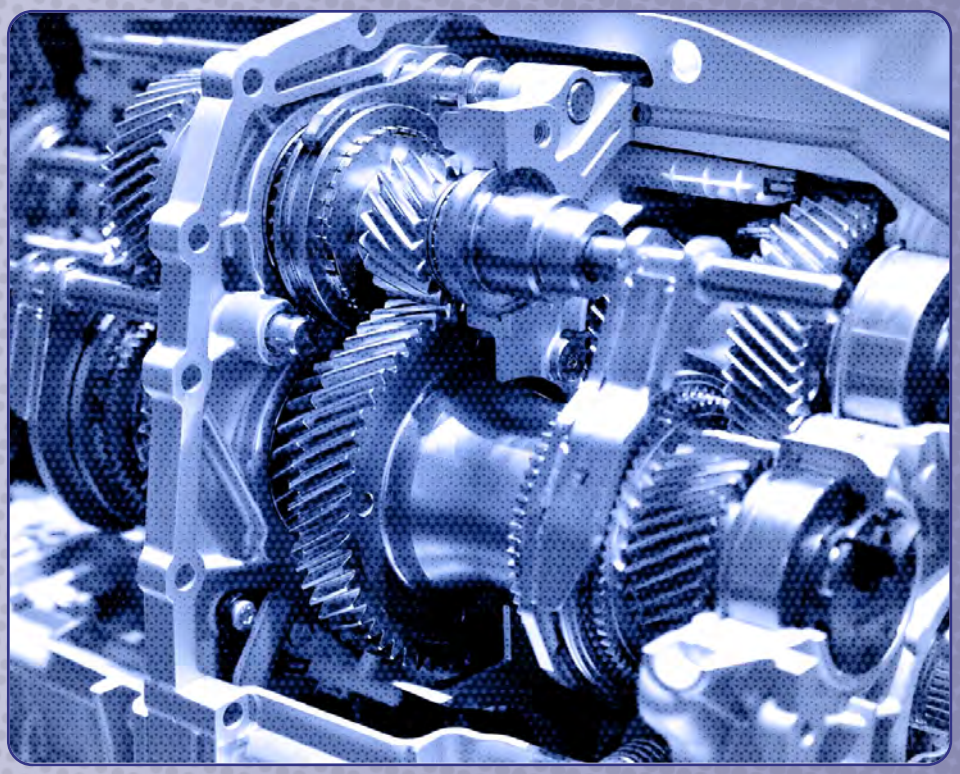

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kenozsir
משחת ט'בה
smörjfett
lubricating grease

Congratulations

Ben Fry

Winner of the 2025 ELGI AGM Best Paper Award

ELGI Awards Committee unanimously selected the Presentation on **"SiToLub - Simulation Tools for the Design of Safe and Sustainable Lubricants"** For the 2025 Best Paper Award Presented by Ben Fry - R.S.Clare / SiToLub Consortium at the 35th ELGI AGM Copenhagen Denmark 2025

All the presentations were evaluated on several criteria that covered the Content of the Paper; Quality of the Presentation and Embodied the Spirit of Originality & Technological Innovations

On behalf of this committee and the ELGI board we would like congratulate Ben Fry on this important and worthy achievement.

Dr Ben Fry is a grease development chemist at RS Clare & Co Ltd. He received a PhD in tribology from Imperial College, London in 2020 studying the friction reducing mechanism of lubricant additives. Since joining RS Clare he has been involved in developing greases for a variety of different applications and is the lead participant for RS Clare on the SiToLub project.

SiToLub - Simulation Tools for the Design of Safe and Sustainable Lubricants

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 requirements 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. It will help the lubricant manufacturers and industrial lubricant users 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, product carbon footprint (PCF) and lifecycle analysis (LCA), and to simulate properties and the interactions within the application environment, to estimate life-time product performance and efficiency during use phase of the new formulations. This paper will address the aims of SiToLub, suggesting how this tool will be used to speed up and improve the formulation of new greases and lubricants and show some initial results from the different models.

SiToLub - Simulation Tools for the Design of Safe and Sustainable Lubricants

Presented at the 2025 ELGI AGM Copenhagen Denmark

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SiTOLUB
SIMULATION TOOLS FOR THE DESIGN OF SAFE AND SUSTAINABLE LUBRICANTS

As part of the European Green Deal,[1] the European Union introduced the Chemical Strategy for Sustainability (CSS)[2] to achieve a toxic-free environment by strengthening regulations, fostering the development and adoption of safer and more sustainable chemicals. The strategy seeks to protect both human health and the environment while ensuring the continued competitiveness of the chemical industry. A key voluntary component of the CSS is the Safe and Sustainable by Design (SSbD) framework,[3] which supports product developers in integrating safety and sustainability considerations into the design of novel chemicals through a more holistic and structured approach. This methodology aims to substitute and eliminate 'Substances of Concern' by addressing human safety, environmental safety, as well as environmental, social and economic sustainability, not only during the manufacturing phase but throughout the entire product lifecycle to highlight trade-offs and to avoid regrettable substitutions.

Proper implementation of SSbD guidelines in a new lubricant's development or during re-design of an existing lubricant requires development chemists to collaborate with a broader range of experts across multiple disciplines, including regulatory affairs, sustainability, purchasing, and supply chain management, as well as key stakeholders such as end users, production teams, sales, and marketing. Therefore, while adhering to SSbD principles ensures that safety and sustainability are addressed simultaneously, it also increases the number of contributors involved in product development, making the process more cost-intensive and potentially slowing down innovation and the introduction of new products to the market.

To overcome these challenges, the SiToLub project, funded under the HORIZON-CL4-2023-RESILIENCE-01 topic, aims to support product developers in applying the SSbD framework by providing computational tools for pre-assessment of lubricant components (base oils, additives, formulations).

The developed models will predict safety (toxicity, biodegradability), performance aspects (properties, stability, tribology), and overall sustainability (LCSA) of the lubricant.

The SiToLub modelling platform will be supported by Artificial Intelligence (AI) functionalities aiming to identify safer sustainable alternatives for the users' requirements and to support the multi parameter decision making process which this involves. SiToLub aims to support a time and cost-efficient pre-screening approach, not only to ensure compliance with current regulatory requirements, but also future-proofing novel formulations against potential regulatory changes.

This paper explores the various models integrated into the SiToLub platform and demonstrates how they can be utilised to assess 'Substances of Concern' across diverse use cases.

Safety Modelling

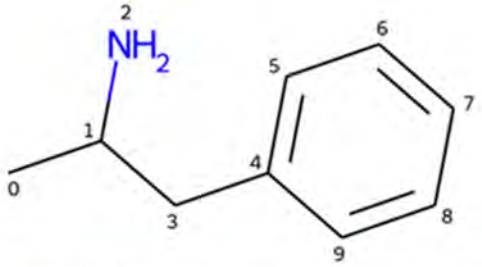
Ensuring both human and environmental safety is a top priority in assessing chemicals, particularly within the Safe and Sustainable by Design (SSbD) framework. However, to properly evaluate both new and existing chemicals on the market, a significant amount of data is needed. At the same time, ethical concerns have led to a major reduction in animal testing (*in vivo*), as society places increasing value on animal welfare[4]. While these two goals - ensuring safety through thorough testing and reducing animal experiments - may seem at odds, researchers are turning to innovative solutions to address both. One of the most promising approaches is the use of *in silico* (computer-based) techniques, which allow scientists to predict the properties of chemicals without the need for live animal experiments.

These methods are widely used in various fields of computational chemistry, particularly in drug discovery and toxicology, where they help predict how chemicals might behave in biological systems or whether they could be harmful[5]. Beyond these fields, *in silico* methodologies are integral to the Safe and Sustainable by Design (SSbD) assessment framework[3], and their implementation facilitates the essential data gap-filling required to complete the assessment, reducing the need for more experiments.

In general, compared to experimental testing, computational predictions offer the advantages of enhanced speed and reduced costs, presenting a more efficient alternative for assessing chemical properties.

Among these computational techniques, QSAR modelling is one of the most promising options[6]. QSAR models (Quantitative Structure-Activity Relationship) rely on mathematical algorithms that, using existing experimental data, can correlate the property with the structure of the chemicals, allowing the prediction of unknown properties of compounds.

The process involves describing chemicals using numerical "descriptors" that capture key structural features. These descriptors can be simple—such as counting specific types of atoms in a molecule—or more complex, measuring aspects like molecular shape, size, or electronic properties, as illustrated in Figure 1.



DESCRIPTOR	Meaning	Value
nBenz	Number of benzene group	1
nN	Number of N	1
nC	Number of C	9
logKow	Partition coefficient octanol/water	1,76
Npath_7	Number of walks of 7 nodes	9

Figure 1, an example of different types of molecular descriptors of a molecule.

Another advantage of QSAR among the *in-silico* models is their regulatory acceptance. Some regulatory bodies, such as REACH, accept the results coming from these models if they fulfil a series of rules established by the OECD[7]. These requirements demand that all relevant information about the model and the obtained prediction to be made available to demonstrate the robustness and reproducibility of the QSAR models[8]. More specifically, these rules state that i) the endpoint modelled should be well-specified, e.g., if a model viscosity is done with data at 25ºC, it will give, as an output, a viscosity value at 25ºC; ii) the algorithm used should be unequivocal, ensuring the reproducibility of the model; iii) proper metrics for the model should be supplied, assuring the robustness and the predictive power of the model; iv) the applicability domain should be well established to know if the analysed chemical fits inside the chemical space covered by the model, ensuring the reliability of the prediction; and v) as far as possible, the results should be accompanied by clear mechanistic interpretations, providing insights into the underlying processes and interactions that drive the observed phenomena.

Within the SiToLub project, QSAR models are being developed following these OECD guidelines. These models will leverage existing experimental data to predict key properties of chemicals, ensuring compliance with regulatory standards. Specifically, SiToLub's QSAR models will assess factors such as human toxicity, ecotoxicity, biodegradability, and other important physical and chemical properties relevant to lubricants and their additives. By integrating these advanced modelling techniques, the project aims to support the development of safer, more sustainable chemicals while reducing reliance on traditional testing methods.

Performance Modelling

The SSbD framework is primarily addressing human and environmental safety, while socio-economic LCA considerations are still underdeveloped, but are being fully investigated within the SiToLub concept. From the industrial perspective, the economic and performance considerations are of the utmost importance. Especially, for the novel alternatives, the performance (functionality) considerations are left for users to be addressed at the design stage. One of the concerns of introducing non-toxic, biodegradable chemicals in the lubricant formulation is their effect on performance. Hence, SiToLub modelling platform integrates into SSbD concept also performance models for uniform benchmarking of existing and new solutions and to enable comprehensive mapping of trade-offs concerning all avenues of safety, sustainability and performance.

Within the performance relevant aspects are physico-chemical properties, thermo-oxidative stability and tribological performance on the molecular and tribological component level, which are addressed by dedicated computational tools. To evaluate these properties, specialised computational tools are used, such as the QSAR models described previously. For example, models are being developed to predict key properties such as viscosity at specific temperatures (e.g., 40°C) and other important attributes like boiling and flash points — factors that influence how base oils and additives perform.

However, to fully understand how lubricants impact machinery efficiency and durability, it is essential to assess how viscosity changes under different conditions, including temperature, pressure, and shear rate. Experimental methods for testing lubricants under such extreme conditions are limited, typically allowing only pairwise measurements (e.g., temperature versus shear rate or temperature versus pressure). SiToLub overcomes this challenge by using advanced molecular simulations, such as non-equilibrium molecular dynamics (NEMD) to predict viscosity behaviour under all these influences simultaneously. This method utilises force fields, such as L-OPLS-AA (Optimised Potentials for Liquid Simulations-All Atom) to model the interactions between atoms, which include terms for bond stretching, angle bending, torsions, and non-bonded interactions such as van der Waals and electrostatic forces. By integrating Newton's equations of motion, classical MD simulations provide insights into the physical movements and interactions of molecules. The collected data are analysed to ensure statistical accuracy and provide input to models assessing performance on the tribological component level, determining frictional losses, among other.

To investigate both how lubricants chemically degrade and the tribological behaviour of the lubricant, the "reactive" molecular dynamics (rMD) simulation enables the capture of the creation and breaking of chemical bonds by employing empirical reactive force fields (ReaxFF) obtained via the density-functional theory (DFT) approach (a quantum mechanical modelling method). Through this, researchers can evaluate and benchmark the stability of lubricants against oxidation and hydrolysis and assess the effectiveness of additives like antioxidants. By constructing tribological gap-alike systems with explicit metallic surfaces, the tribofilm formation and derived CoF values for extreme pressure, anti-wear additives and corrosion inhibitors can be determined under various temperature, pressure and shear rates enabling direct comparison and leading to performance map plots fundamental for “fit-for-application" decision support.

For the assessment on the tribological component level, the Finite Element Method (FEM) approach is pursued to determine: the pressure evolution within tribological contacts; the efficiency (frictional losses) and durability (wear losses) of systems, such as journal bearings, gears, etc.; as well as performance derived from the four-ball tester. The FEM models take into account the contact situation, while considering explicit properties of materials and even of fully formulated lubricants, real topographies, as well as realistic operational conditions.

The input values for the assessment can come from MD and rMD models, from the benchmarking of theoretical candidates, as well as from experimental validation studies with the acquired (bought) most promising candidates. To ensure accuracy, these models are validated against both experimental data and molecular-scale simulations, helping researchers and industries identify the most promising lubricant formulations in terms of expected performance before physical testing.

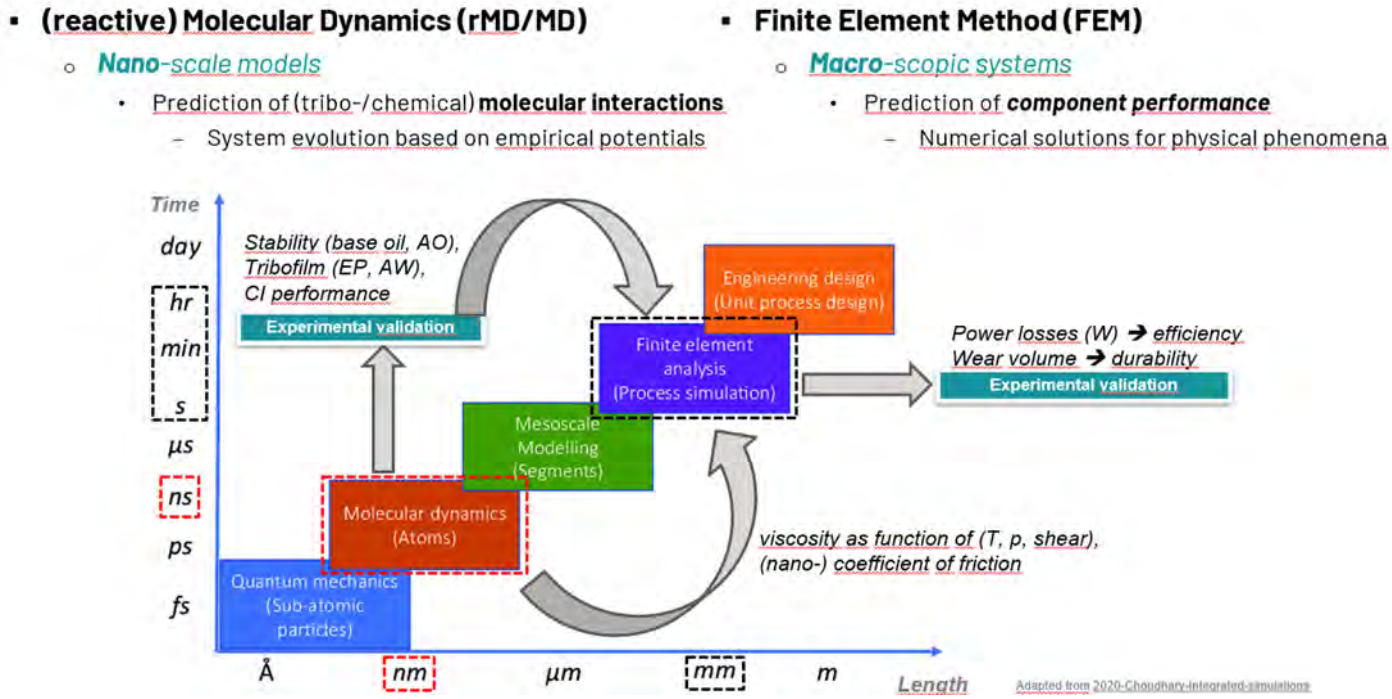


Figure 2, A diagram showing the scales of the different performance models being used in the SiToLub platform.

Sustainability Modelling

As part of the sustainability assessment framework within the SiToLub project and in line with Safe and Sustainable by Design (SSbD) principles, Life Cycle Assessments (LCA) for novel lubricants will be simulated. LCA is based on the concept of Life Cycle Thinking (LCT), which takes a broad perspective, considering all environmental impacts of a product from production to disposal. Unlike the Product Carbon Footprint (PCF), which mainly measures greenhouse gas emissions—often only up to the point a product leaves the factory (cradle-to-gate)—LCA examines a wider range of environmental effects, including toxicity, water use, resource depletion, and ecosystem impacts, throughout the entire life cycle (cradle-to-grave). For example, the Environmental Footprint (EF) method developed by the European Commission's Joint Research Centre assesses environmental impact across 11 main categories and 14 subcategories, some of which are shown in Figure 3. This comprehensive approach helps avoid "burden shifting," where reducing one environmental issue (such as lowering carbon emissions) unintentionally causes another (such as increased resource depletion or land use). This is particularly relevant when switching to renewable materials or energy sources.

Beyond environmental factors, LCA also considers economic and social aspects. The economic dimension is analysed through Life Cycle Costing (LCC), which looks at financial costs across a product's lifespan, while social Life Cycle Assessment (sLCA) examines impacts on people and communities. The SSbD framework promotes a Life Cycle Sustainability Assessment (LCSA), which integrates these three approaches—environmental, economic, and social—to provide a well-rounded evaluation of a product's overall sustainability.

Figure 3, The different environmental effects evaluated within a life cycle assessment of a lubricant.

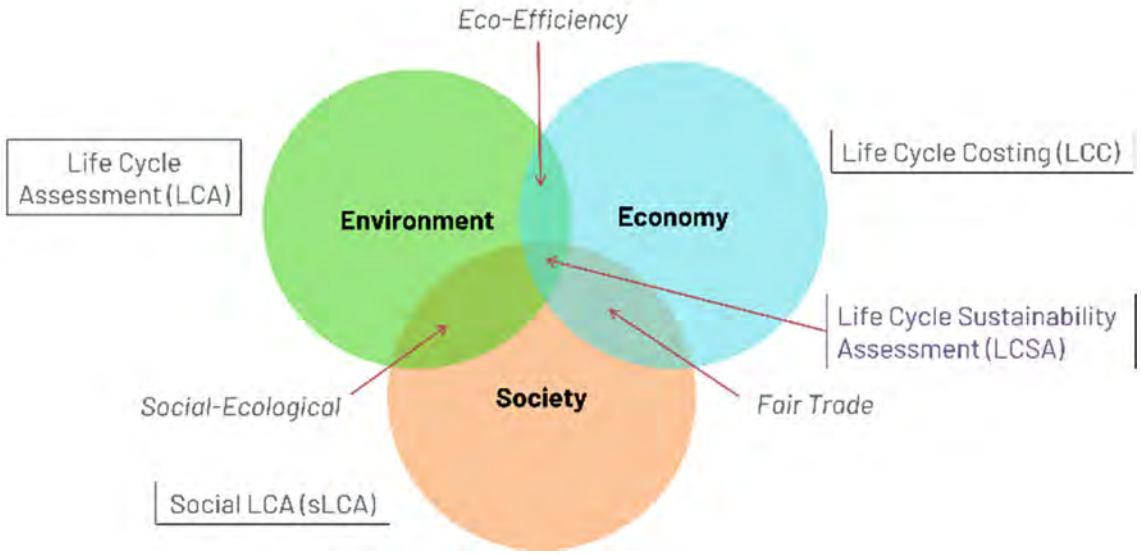


Figure 4, The factors included within a Life Cycle Sustainability Assessment (LCSA).

In this project, we use life cycle models specifically designed for lubricants—materials that play a crucial role in reducing friction and improving efficiency, making them essential for sustainability. These models go beyond simply analysing the raw materials, production, and transportation of lubricants. Instead, they place a strong focus on their use phase, particularly their impact on energy efficiency, as well as their end-of-life options, such as recycling, natural degradation, or incineration. The QSAR models described above will deliver data on (eco)toxicity and biodegradability that can be fed into the life cycle model, combined with the performance assessment tools that provide insight on the functionality of the formulation, which enables the comparison of environmental and socioeconomic impacts. This becomes particularly important because when a lubricant minimises power losses and extends the durability of equipment, the overall environmental impact is significantly reduced.

In that sense, a major advantage of the SiToLub approach is conducting these assessments using simulated data, allowing the development of new lubricants to be sped up, and then also validating these predictions through laboratory experiments, refining the data needed for a more comprehensive life cycle assessment (LCA),

effectively cutting down the development time of novel lubricants within this project. By combining these models with established LCA databases, the SiToLub platform will help identify more sustainable lubricant options with lower environmental and social impacts. In the final stage, a life cycle sustainability assessment (LCSA) will compare the overall sustainability of these simulated lubricants with existing market solutions, providing a well-rounded recommendation of the best alternatives.

The use of AI to assess formulations and develop new molecules

The SiToLub platform will, using the integrated models described above and advanced AI tools, enable users to explore and design new molecular formulations that meet their safety, performance and sustainability standards.

Through a simple questionnaire, users will be able to specify their needs - such as removing harmful substances like PFAS or chlorinated paraffins - and define key performance criteria, including stability, durability, and environmental impact. Based on all these inputs, the SiToLub AI model will identify suitable candidate molecules as alternatives to the lubricant components that the user wants to replace. The so called SiToLub Molecule Designer will identify replacement candidates within the SiToLub database and associated catalogues based on similarity to known molecules that meet all or most user requirements. The AI also produces a ranking based on how many of the users' criteria the individual candidates meet.

The molecule candidates suggested by the SiToLub AI can then be compared to each other by assessing their performance, sustainability, and safety with the SiToLub models. Users will then be supported to prioritise safety, sustainability, and performance parameters by clearly identified trade-offs and defined weighting criteria within Multi-Criteria Decision Analysis (MCDA)[9].

Beyond identifying replacements, SiToLub also intends to offer an Explorative AI model for those looking to rethink lubricant formulation at a deeper level. Trained on comprehensive data about chemical functions and reactions, the Explorative AI will be tasked to recognise the implicit guiding principles behind inter-molecular chemical reactions. Based on that holistic chemical understanding, the explorative AI will suggest wholly original – yet plausible – replacement candidates. These can be tested, too, and further AI tools are planned to give formulators an indication of how to source and/or produce these novel molecules.

Validation of the toolbox via use cases

The SiToLub platform is being developed to help create more sustainable and safer lubricants. To ensure its effectiveness, the platform will be tested and validated on real-world industry challenges, focusing on the replacement of chemicals that are under regulatory scrutiny due to their environmental and health impacts. Operatively, the project will focus on finding alternatives for some of the most concerning substances:

1. PFAS (Per- and Polyfluoroalkyl Substances)

PFAS chemicals are commonly used in lubricants for their durability and resistance to extreme conditions. However, both in European legislation[10] and lubricants industry[11] literature they are often referred as "forever chemicals" because they do not break down easily in the environment and have been linked to health concerns, including endocrine disruption. This consideration drove a demand for removal by the EU and an active commitment by the industry to seek and/or develop suitable replacements. The SiToLub project will specifically study PTFE (used as an anti-wear additive) and PFPE (a stable base oil).

2. Chlorinated Paraffins

Short chained, chlorinated paraffins are used as extreme pressure additives within oil-based metal working fluids, specifically for the metal stamping process. These molecules are classed as persistent organic pollutants and require special end of life treatment to avoid toxic degradation products[12]. The project will explore alternative additives that offer similar performance without the environmental drawbacks.

3. Benzotriazole

There are a limited number of sustainable corrosion inhibitors available to the market, as shown by the number available on the LuSC list for EU Ecolabel.[13] Benzotriazole is a widely used corrosion inhibitor and metal deactivator but is also toxic for reproductive functions, toxic to aquatic life and a suspected endocrine disruptor[14].

SiToLub will investigate safer substitutes that still provide effective corrosion protection.

Finding viable replacements for these chemicals is a high priority for both lubricant manufacturers and additive suppliers. Hence, supporting the development of the platform and its continuous improvement through regulatory and industrial evolution would ensure long-lasting efficiency and benefits. If time allows, further chemistries such as diphenylamine antioxidants and phosphorothionate anti-wear additives will also be tested on the platform to find more sustainable alternatives.

Validation of the computational tools

The models developed during the SiToLub project will undergo validation in two phases: first, by the project partners, and then by external stakeholders. To facilitate this, an Open Call for Early Adopters will be launched, inviting interested users to be among the first to utilise the cutting-edge tools that will be progressively released throughout the project. If you are already interested, please contact us at info@sitolub.eu.

Beyond the SiToLub project duration

The SiToLub project runs from January 2024 to December 2027, with the goal of creating a fully validated digital platform for lubricant formulation. However, for the platform to remain available beyond the project's duration, it must be integrated into a sustainable business model. In that regard, i-TRIBOMAT: The European Tribology Centre, will host and nurture the SiToLub toolbox by integrating the models resulting from the SiToLub project to the already available Tribology Universe platform. One example is the recently launched calculator app, which predicts a lubricant's viscosity and density across a wide range of pressures and temperatures. This app marks the first of many tools to be released as part of the SiToLub project and is available for free to anyone with an internet connection via the Tribology Universe platform (see Figure 5).

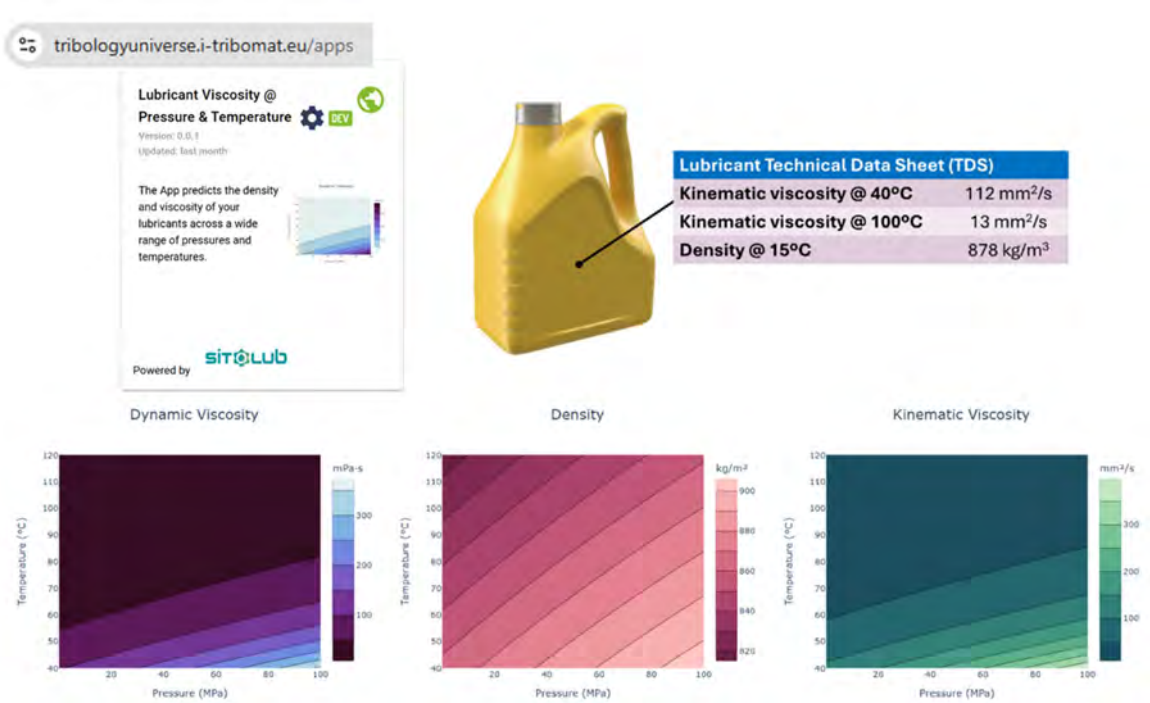


Figure 5, Application for predicting a lubricant's viscosity and density across a wide range of pressures and temperatures (Tribology Universe, www.i-tribomat.eu).

The support and hosting of SiToLub on the i-TRIBOMAT platform will ensure that the tools remain online and operational, while i-TRIBOMAT will also promote their use through its academic and industrial network.
To find out more about the project and to sign up to our newsletter for further updates please visit our website. https://sitolub.eu/

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