



sitolub

THE SITOLUB TOOLBOX

Your AI-powered
lubricant formulator
and selector assistant



Co-funded by
the European Union

USER JOURNEYS

● Molecular Lubricant Design

1) Substance replacement

2) Virtual evaluation

- A1 GenAI molecular designer
- A2 Biodegradability & (Eco)toxicity
- A3 Physico-chemical properties
- A4 Stability prediction
- A5 Tribofilm prediction
- A6 Compounds database
- A7 Toxicity database
- A8 Product Carbon Footprint tool
- A9 SSbD benchmarking



● Rheology

- B1 Full rheological characterisation
- B2 Virtual property prediction
- B3 Rheological model fitting
- B4 Rheology comparer
- B5 Viscosity blend calculator
- B6 Artificial ageing



● Lubricant Applications

- C1 Testing & benchmarking
- C2 Journal / Spiral bearing
- C3 Transmission gear
- C4 Metal Working Fluid
- C5 Tribology database
- C6 Spiral groove thrust bearing
- C7 Tilting-pad thrust bearing



● Compliance

- D1 LCSA database
- D2 ESPR / Digital Product Passport
- D3 SSbD consultancy



3) Lubricant comparison	4) Application performance	5) Stability & service life	6) Sustainability & compliance
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MOLECULAR DESIGN

APP

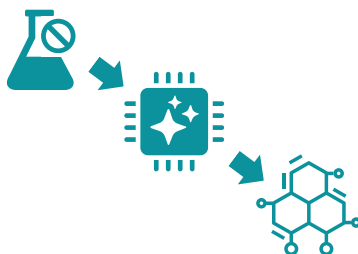
Lubricant Formulator

Additive Manufacturer

A1 GenAI molecular designer

AI-powered molecular designer **specific for lubricant** to obtain **safer, sustainable and high performing lubricant alternatives**.

First-level shortlist of viable safe, sustainable, high-performing candidates, for detailed SSbD assessment and/or experimental validation steps.



APP

Lubricant Formulator

Additive Manufacturer

Base Oil Producer

A2 Biodegradability & (Eco)toxicity

Predicts **(eco)toxicity, biodegradability and SVHC** for lubricant components from molecular structure. Time and cost-efficient to **screen large ingredient lists in minutes**, to eliminate acquisition and experimental tests while supporting regulatory submissions.



APP

Lubricant Formulator

Additive Manufacturer

Base Oil Producer

A3 Physico-chemical properties

Predict additive's surface protection capabilities for **EP, AW, FM and corrosion inhibitor** candidates and obtain insights for CoF values, surface protection against water and salt, in dependence of applied T,

pressure, shear rate. Avoid costly trial-and-error testing and **select promising candidates early**, to enhance your formulation performance.

SERVICE

Lubricant Formulator

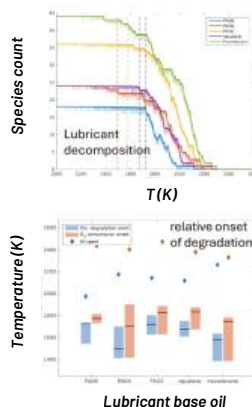
Additive Manufacturer

Base Oil Producer

A4 Stability prediction

Utilize reactive MD insights to rank base oil candidates by their **resistance to thermal-oxidative and hydrolytic degradation**.

Obtain e.g., degradation onset temperatures, main degradation products in dependence of applied T, pressure, shear rate as well as in presence of nascent catalytic surface, contaminants, and different atmospheres prior tests.



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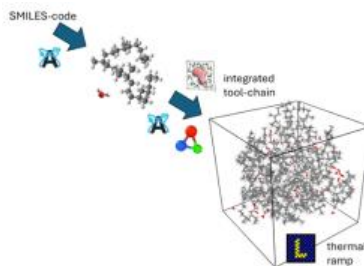
Lubricant Formulator

Additive Manufacturer

Base Oil Producer

A5 Tribofilm prediction

Uses reactive molecular dynamics simulation to predict, at the atomic level, whether an **EP, AW, CI, or FM additive candidate will form a protective tribo-film on a target metal surface** – ranking candidates by film quality and stability before any tribometer test is run.



SERVICE

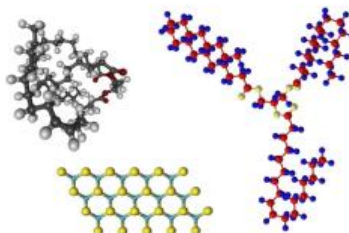
Lubricant Formulator

Additive Manufacturer

Base Oil Producer

A6 Compounds database

A growing database of **chemical, (eco)toxicological, and biodegradability data** for substances relevant to **lubricant formulation**. Provides the reference data needed for hazard screening, substitution searches, and regulatory reporting.

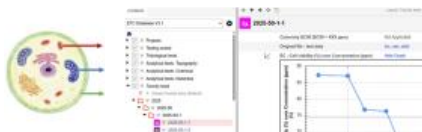


DATASET

Additive Manufacturer

A7 Toxicity database

Experimental ecotoxicity and cytotoxicity data for **lubricant-relevant chemicals**.



APP

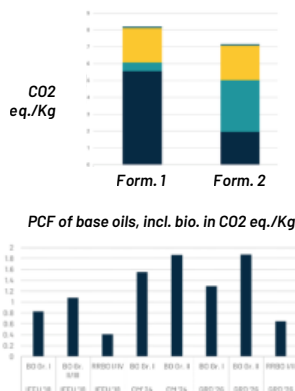
Additive Manufacturer

Lubricant Formulator

A8 Product Carbon Footprint tool

Calculates the **product carbon footprint** (cradle-to-gate, ISO 14067-aligned) of a lubricant formulation recipe, with **component-level hotspot breakdown** and side-by-side comparison between alternative recipes.

Gives R&D teams **estimated carbon footprint data** to reduce the carbon impact of a formulation before it leaves the lab, and to respond to OEM or retailer requests.



APP

Lubricant Formulator

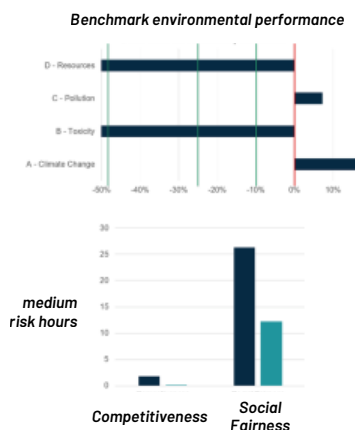
Additive Manufacturer

Base Oil Producer

A9 SSbD benchmarking

Assesses whether a candidate lubricant formulation or additive is not only safer and higher-performing, but also more sustainable – benchmarking it against a **reference** solution across **environmental**, **economic**, and **social dimensions** under the SSbD framework.

Flags CRM and SVHC usage and identifies the key impact hotspots.



RHEOLOGY

SERVICE

Lubricant Formulator

Additive Manufacturer

Base Oil Producer

OEM/Component manufacturer

B1 Full rheological characterisation

Delivers a **comprehensive experimental viscosity and density map** across wide range of pressures, temperatures, and shear rates – including the pressure-viscosity coefficient.

Provides high-quality input data to feed and validate **simulation models** and to **objectively benchmark** base oils and lubricants.



SERVICE

Lubricant Formulator

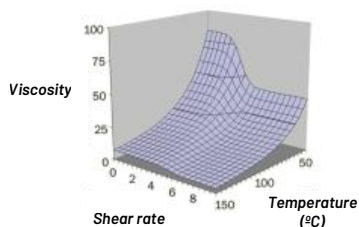
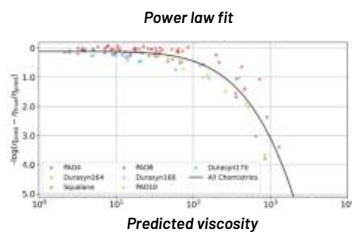
Additive Manufacturer

Base Oil Producer

OEM/Component manufacturer

B2 Virtual property prediction

Fits rheological models to experimental and/or MD-derived viscosity data to obtain so-called Master curve to predict **viscosity at any T-p-shear rate combination**. Turns raw measurement data into a ready-to-use **predictive model for benchmarking, simulation model feed and to support lubricant formulation**.



SERVICE

Lubricant Formulator

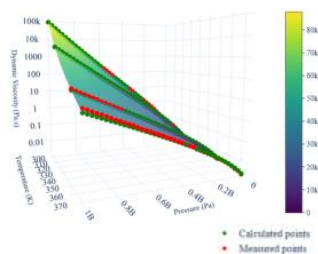
Additive Manufacturer

Base Oil Producer

OEM/Component manufacturer

B3 Rheological model fitting

Fits rheological models to experimental and/or MD-derived viscosity data to obtain so-called Master curve to predict **viscosity at any T-p-shear rate combination**. Turns raw measurement data into a ready-to-use **predictive model for benchmarking, simulation model feed** and to support **lubricant formulation**.



Shear rate dependency



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Lubricant Formulator

Additive Manufacturer

OEM/Component manufacturer

Base Oil Producer



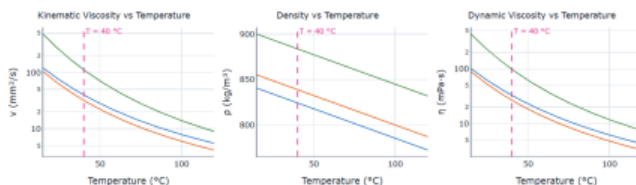
B4 Rheology comparer

Benchmarks **fresh or aged lubricants** side-by-side with interactive viscosity plots across user-defined **temperature, pressure and shear rate ranges**, utilizing fitted rheological model.



Lubricant Technical Data Sheet (TDS)	
Kinematic viscosity @ 40°C	112 mm ² /s
Kinematic viscosity @ 100°C	13 mm ² /s
Density @ 15°C	878 kg/m ³

Replaces manual datasheet comparisons with customizable visual outputs for conditions of interest.



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Lubricant Formulator

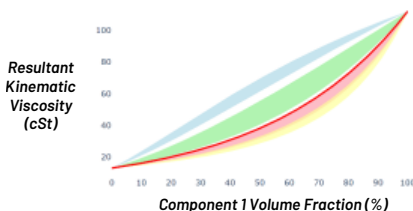
Base Oil Producer



B5 Viscosity blend calculator

Predicts the **kinematic viscosity** of a two-component lubricant blend before mixing using the **Lederer-Roegiers equation**.

Reduces formulation trial-and-error by giving an instant estimate before any physical blending takes place.



SERVICE

Finished Lubricant Formulator

Additive Manufacturer

Base Oil Producer

OEM/Component manufacturer

B6 Artificial ageing

Artificial ageing of lubricants under controlled temperature, pressure and **atmosphere (O₂, H₂, CH₄, N₂ or combinations)** to simulate in-service degradation, using standardised protocols (CEC L-48-A-95, RULER).

Contaminants can be introduced deliberately – water, salt and catalytic metals such as copper – to reproduce the degradation drivers of marine, offshore and industrial service.

Generates degradation profiles and kinetics to validate stability predictions and support reformulation.



LUBRICANT APPLICATIONS

SERVICE

Finished Lubricant Formulator

Additive Manufacturer

Base Oil Producer

C1 Testing & benchmarking

Lab-scale and component-level testing of lubricants and greases covering friction, wear, oxidation and load-carrying capacity (FZG, FE8, FE9, four-ball, SRV, HFRR, RPVOT and more), **benchmarked against reference lubricants in the European Tribology Centre database.**



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Finished Lubricant Formulator

Additive Manufacturer

OEM/Component manufacturer

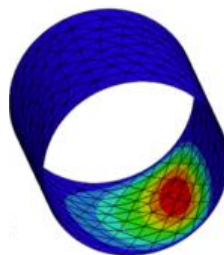
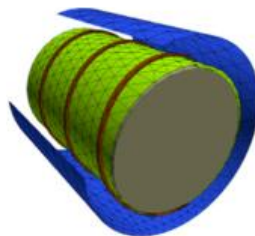
Base Oil Producer



C2 Journal / Spiral bearing

Predicts **frictional losses (efficiency)** and **wear volume (durability)**, among other, resulting from contact situation and operating conditions of tailored contact geometry model for customer's lubricant and material pairing use-case.

Enables time- and cost-efficient performance prediction to optimize **lubricant formulation and/or bearing design.**



Lubricant pressure (MPa)



SERVICE

Lubricant Formulator

Additive Manufacturer

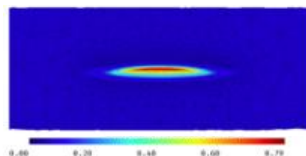
OEM/Component manufacturer

Twin-disc model

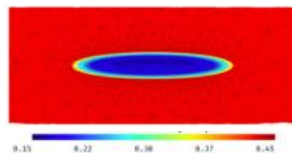
**C3 Transmission gear**

Predicts **frictional losses (efficiency)** and **wear volume (durability)** under **boundary-to-mixed regime** under various **SRR conditions**, among other, resulting from accurate lubricant rheology and material (geometry, composition, roughness) pairing under test-rig conditions.

Time- and cost-efficient performance prediction to **optimize AW selection and design**.



Lubricant pressure



Lubricant gap

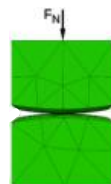
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Lubricant Formulator

Additive Manufacturer

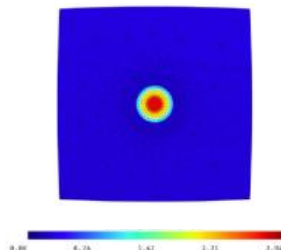
OEM/Component manufacturer

4-ball model

**C4 Metal Working Fluid**

Models **boundary lubrication performance for metalworking fluids** – the thin-film, asperity-contact regime that governs friction, wear and surface finish across cutting, milling, forming and stamping operations.

Uses **four-ball / sliding contact geometry** to predict wear scar, friction coefficient and load-carrying capacity for when the full fluid film breaks down, enabling ranking of wear resistance and **EP additive selection**.



Contact pressure



Wear

DATASET

Finished Lubricant Formulator

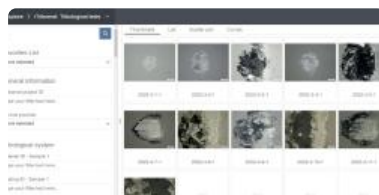
Additive Manufacturer

Base Oil Producer

OEM/Component manufacturer

C5 Tribology database

Reference **experimental wear, friction, and efficiency data for lubricants** under a wide range of operating conditions. Provides **benchmark data** to validate simulation models and support performance claims.



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Lubricant Formulator

Additive Manufacturer

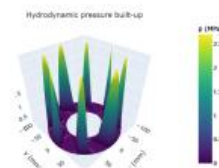
OEM/Component manufacturer

Base Oil Producer



C6 Spiral groove thrust bearing

Models the **load-carrying capacity, film thickness, and friction torque** of a spiral-groove thrust bearing from the lubricant properties and the groove geometry — aimed at high-speed, precision, low-load applications.



Hydrodynamic pressure

APP

Lubricant Formulator

Additive Manufacturer

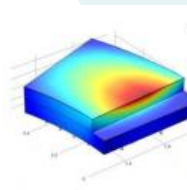
OEM/Component manufacturer

Base Oil Producer



C7 Tilting-pad thrust bearing

Predicts the **hydrodynamic performance of a tilting-pad thrust bearing** — load carrying capacity, minimum film thickness, and friction loss — from the lubricant rheology together with the pad geometry and duty cycle.



Hydrodynamic pressure

COMPLIANCE

DATASET

Finished Lubricant Formulator

Additive Manufacturer

Base Oil Producer

D1 LCSA database

Lubricant LCSA database provides **curated LCA datasets for base oils and 80+ additives** in **ILCD or CSV format**, filling the gaps left by generic databases for lubricant chemistries.

Where a substance is not yet covered, **we model it from scratch – no formulation is left without a sustainability data foundation.**



SERVICE

Finished Lubricant Formulator

Additive Manufacturer

Base Oil Producer

D2 ESPR / Digital Product Passport

Aggregates the safety, sustainability and performance data generated across SiToLub workflows into a **structured, machine-readable Digital Product Passport (DPP)**.

Ready for customer sharing, supply chain integration or regulatory submission – **be ESPR-ready before the DPP becomes mandatory.**

SERVICE

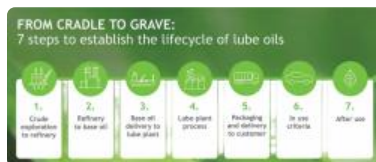
Finished Lubricant Formulator

OEM/Component Manufacturer

D3 SSbD consultancy

Expert-led life cycle sustainability study for lubricant formulations and additives, combining environmental, economic, and social assessment perspectives in a **structured SSbD-aligned workflow.**

Delivers a **benchmark comparison, hotspot analysis, and design recommendations** – from early screening to detailed comparative studies.



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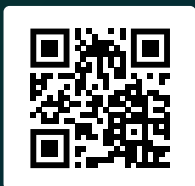
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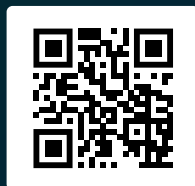
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