

# Simulation Tools for the Design of Safe and Sustainable Lubricants

SITOLUB

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# VGP 2013 & EALs

## What is an Environmentally Acceptable Lubricant (EAL)?

- Biodegradable
- Minimally toxic
- Not bioaccumulative

## Is "coffee" an EAL?

## VGP suggestion on base oils...

- Synthetic Esters (HEES)
- Polyglycols (HEPG)
- Poly- $\alpha$ -olefins (HEPR)
- Triglycerides (HETG)

## What is VGP?

Vessel General Permit is a regulation put in place to stop harmful lubricant discharge and its impact on U.S. waterways.



Applies to vessels that are 79 ft or greater in length

Covers all U.S. waters, including seaward from coasts & Great Lakes up to **3 MILES**

**Deck**  
Suggested

**Below waterline**  
(oil-to-sea interfaces)  
Required



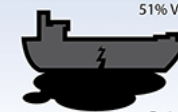
61,000 U.S. ships subject to VGP

(EPA estimates)



8,000 Foreign ships subject to VGP

### Top 5 Inputs of Lubricants in World's Marine Port Waters



51% Vessel Operational Discharges  
19% Tank Ship Spills  
10% Lube Leakages  
7% E&P Produced Waters  
7% Tanker Cargo Washings

Estimated annual total discharge:  
37-61 M liters (10-16 M gallons)

## What is an EAL?

An environmentally acceptable lubricant (EAL) is a VGP compliant lubricant.

EALs are:

- biodegradable
- minimally toxic
- not bioaccumulative

... as defined in Appendix A of the 2013 VGP



### EAL Base Oil Selections

- Soybean, canola, sunflower plus blends
- Other vegetable matter base stocks
- PAGs
- Synthetic esters



### VGP affects a wide range of equipment

- Wire rope
- Stern tubes
- Controllable pitch propellers
- Azipods
- Rudder bearings
- Stabilizers
- Thruster azimuth bearings
- Thruster hydraulic fluids
- Mechanical equipment subject to immersion



# VGP 2013 & EALs

## It needs to be an “Environmentally Acceptable Lubricant”

- Biodegradable
- Minimally toxic
- Not bio-accumulative

TEST / MODEL



## It needs to “mechanically” work!

- Viscosity
- Density

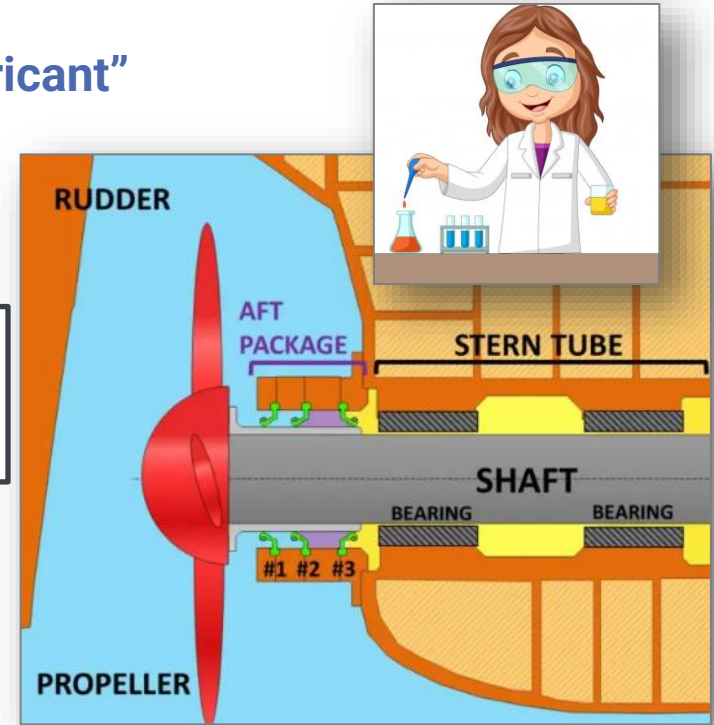
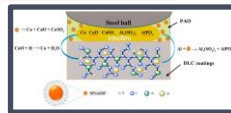
TEST / MODEL



## It needs to “chemically” work!

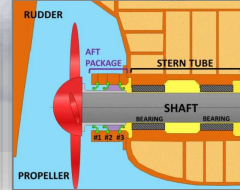
- Hydrolysis
- Oxidation
- Compatibility

TEST / MODEL



# VGP 2013 & EALS

## Fluoroelastomers (FKM)



### It needs to be an “Environmentally Acceptable Lubricant”

- Biodegradable
- Minimally toxic
- Not bio-accumulative

TEST / MODEL



### It needs to “mechanically” work!

- Viscosity
- Density

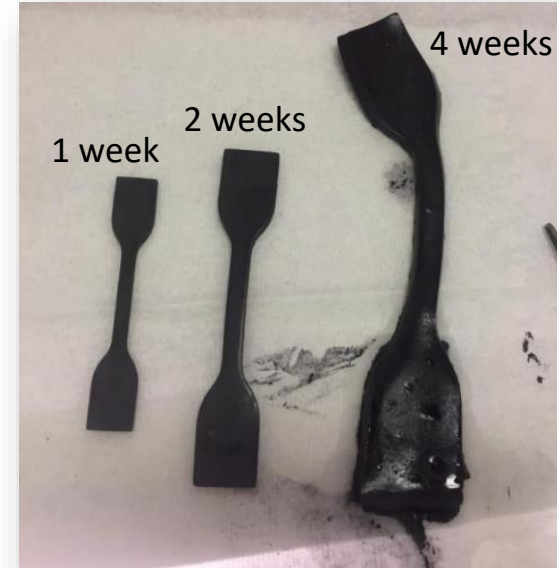
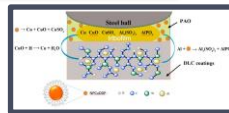
TEST / MODEL



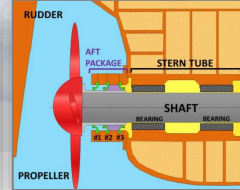
### It needs to “chemically” work!

- Hydrolysis
- Oxidation
- **Compatibility**

TEST / MODEL



## Fluoroelastomers (FKM)

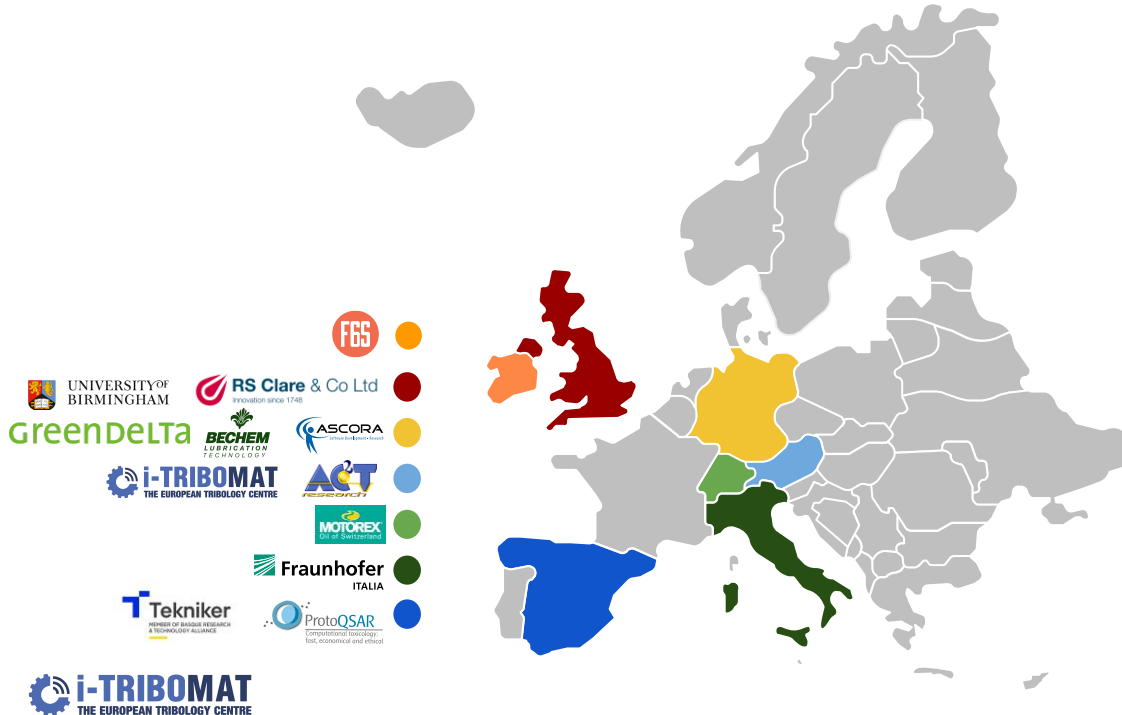


contamination  
water repellent PFAS PFOA PFOS  
chemical compounds forever chemicals  
Water Pollution toxic and carcinogenic  
biochemistry cancer polyfluoroalkyl waterproof PFAS Human health impermeable warning  
environmental damage  
Perfluoroalkyl and Polyfluoroalkyl  
water-resistant properties  
organofluorine fluorochemicals  
PFAS exposure

### Development of computational models to facilitate the formulation of lubricants

...to overcome the challenge posed to the industry by

- new market demands
- regulatory requirements
- shortage of raw materials



**SITOLUB**

<https://sitolub.eu/>

Jan 2024 - Dec 2027

# i-TRIBOMAT: The European Tribology Centre

## Industry

“bring new products to market faster”



Manufacturer

### Needs

- 1) Tribological tests
- 2) Data driven
- 3) Simulation
- 4) Knowledge

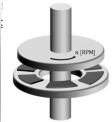
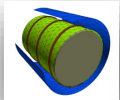
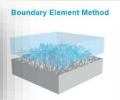
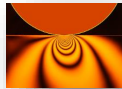


**i-TRIBOMAT**  
THE EUROPEAN TRIBOLOGY CENTRE



**Tribology Universe™**

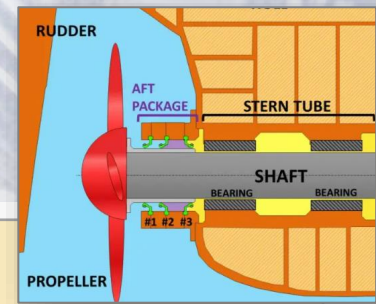
Database  
Online Apps



## Service Providers



# Where do we stand?



**Database**  
**i-TRIBOMAT**  
 THE EUROPEAN TRIBOLOGY CENTRE

- Materials/Lubricants**
- Wear rate
  - Friction coefficients
  - Composition
  - Toxicity
  - Biodegradability
  - LCA

**Tribology Universe™**

**Geometry**  
**Material properties**  
 viscosity, density  
**Surface finish**  
**Operating conditions**  
 Velocity  
 Load

→

**Journal Bearing App**

→

**Film thickness**  
**Pressure build-up**  
**Contact force**

**QSAR**

→

**Toxicity model**  
**Biodegradability model**  
**Life Cycle Assessment**  
**Compatibility**

→

**Toxicity level**  
**Biodegradability**  
**Carbon footprint**  
**Go/ no-Go**

**Generative AI-model**

- Which off-the-shelf lubricant should I use?
- Which formulation can fulfill the requirements of the application?



# Generative AI challenge



Manufacturer

UI: How Users Could Input Prompts

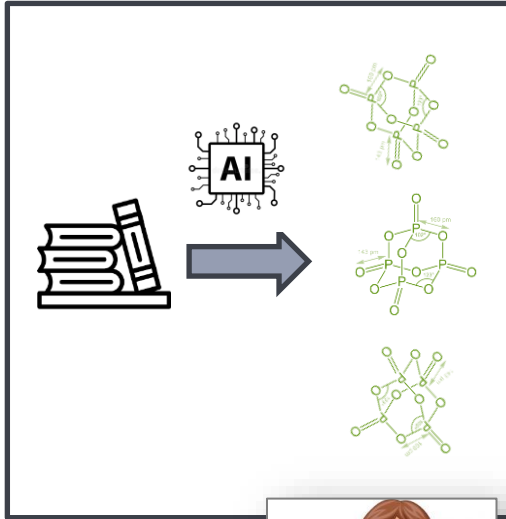
- LABEL X1
- ECO LABEL
- LABEL X2
- LABEL X3

- |   |  |
|---|--|
| <input checked="" type="checkbox"/> Performance | <input type="checkbox"/> Only Natural Products |
| <input type="checkbox"/> Sustainability         | <input type="checkbox"/> Criteria X1           |
| <input type="checkbox"/> Toxicity               | <input type="checkbox"/> Criteria X2           |
| <input checked="" type="checkbox"/> Price       | <input type="checkbox"/> Criteria X3           |

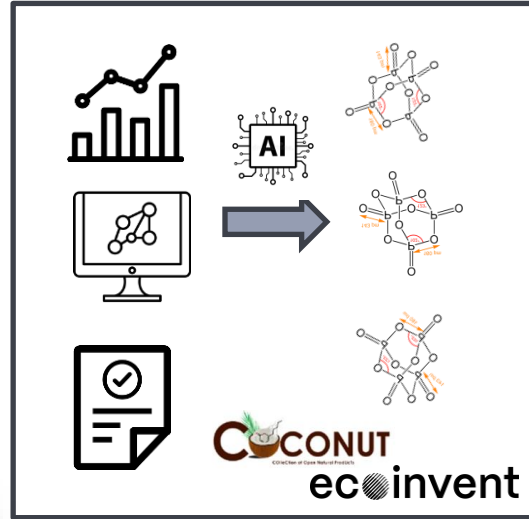
- |   |   |
|---|---|
| <input type="checkbox"/> Chemical X1            | <input type="checkbox"/> Chemical X5            |
| <input checked="" type="checkbox"/> Chemical X2 | <input checked="" type="checkbox"/> Chemical X6 |
| <input type="checkbox"/> Chemical X3            | <input type="checkbox"/> Chemical X7            |
| <input type="checkbox"/> Chemical X4            | <input checked="" type="checkbox"/> Chemical X8 |

# Generative AI challenge

## 1. Generate "candidate" molecules

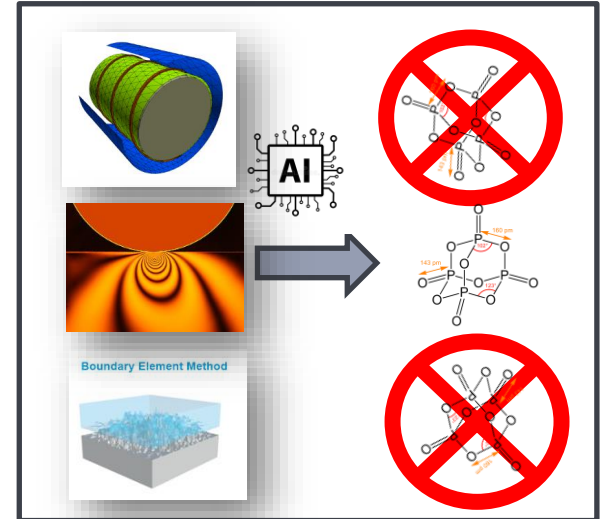


## 2. Find molecules with similar SMILES code

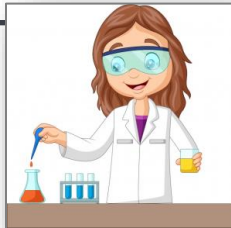


695,000+ individual molecules

## 3. Determine which molecules can fulfill the requirements



List of potential lubricant components.





**Use cases for validation:**

- 1) Elimination of PFAS
- 2) Elimination of Chlorinated paraffins
- 3) Elimination of Li-soaps

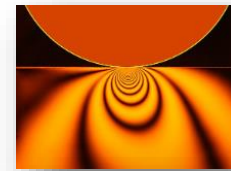
## We are looking for external users

a) [Validate the online models](#) (a few are already available!)

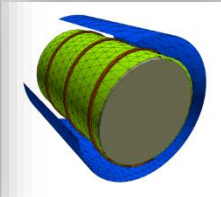
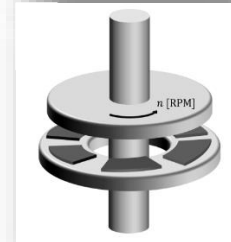
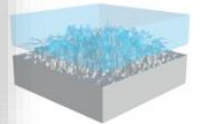
- Testers of the Tribology Universe™ [www.i-tribomat.eu](http://www.i-tribomat.eu)

b) [Validate the novel lubricant formulations](#) (2025-27)

- Testers of AI-formulated lubricants



Boundary Element Method





## AWARDS

- ✓ Winner of the **European Enterprise Award 2023** as *Most Innovative Engineering & Manufacturing Digital Transformation Enterprise*.
- ✓ **1<sup>st</sup> place “riz-up Genius Award 2023”** in the category of *Innovatively Brilliant*.
- ✓ **1<sup>st</sup> place “tecnet | accent Innovation Award 2023”** in the category of *Start-up – innovative, technology-based business ideas*.
- ✓ **3<sup>rd</sup> place** for the **“Digital Impuls Award 2021”** for the *Best Digitalization Project of Austria*