SSbD in process industry

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SITOLUB
SIMULATION TOOLS FOR THE DESIGN OF SAFE AND SUSTAINABLE LUBRICANTS

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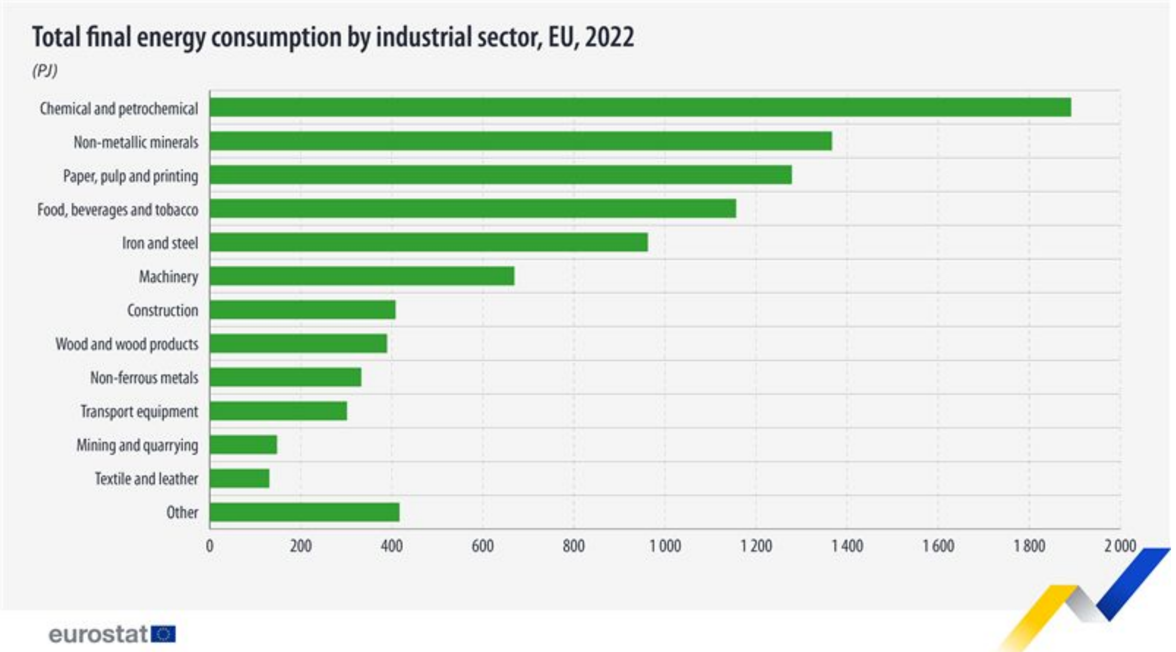
What is the process industry?

- Process industry is a broad term encompassing sectors like chemical, refining, pulp and paper, steel, cement, and other
- These industries handle large quantities of raw materials and produce finished products through various chemical, physical, and biological transformations
- Process industry is the main beneficiary of SSbD materials



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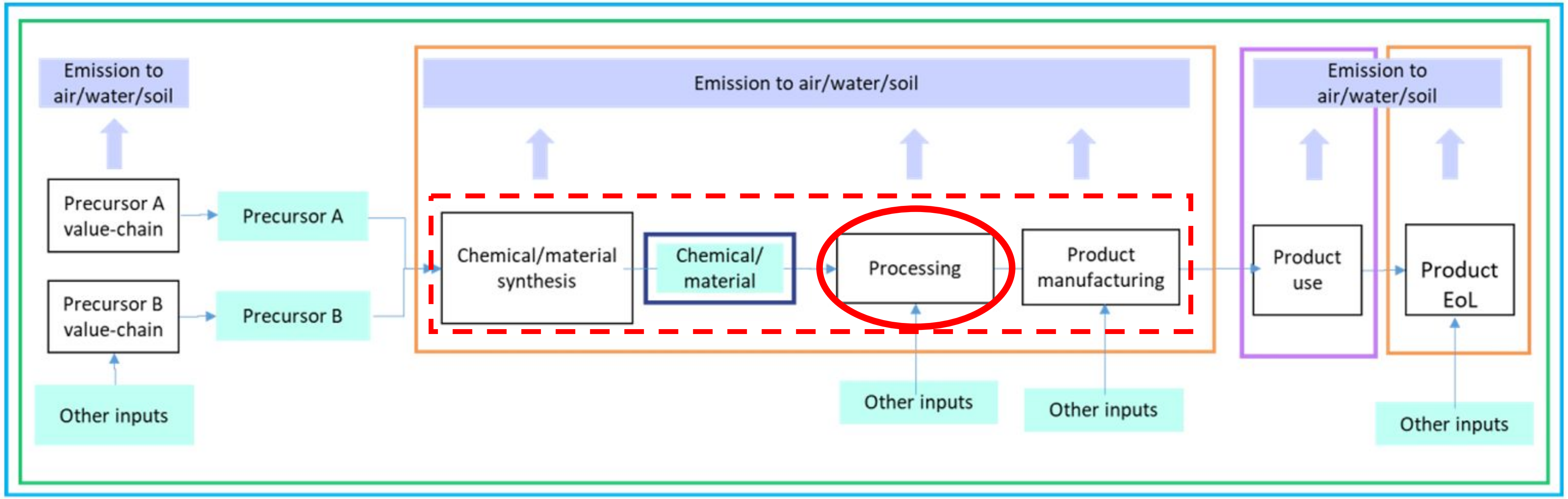
The JRC visualizes the processes as part of the production safety, environmental sustainability and the economic assessment (steps 2, 4 and 5)



- Step 1 - Hazard Assessment
- Step 2 - Human health and safety aspects (production and processing)
- Step 3 - Human health and environmental aspects (final applictaion)
- Step 4 - Environmental sustainability assessment
- Socio - economic assessment

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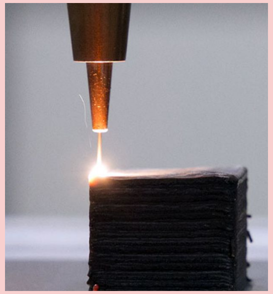
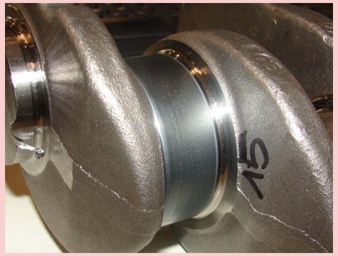
Improving the **safety** dimension of processes

MATERIAL FORMAT: from dust to wire for metal printing

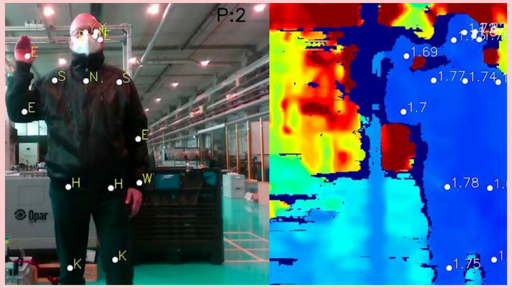


SECONDARY SUBSTANCES: from chemical to physical coatings

PHYSICAL HAZARDS: from bulk to surface treatments



SAFE ENVIRONMENTS: human-machine interaction



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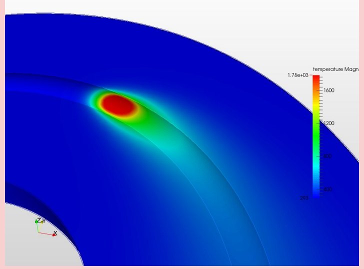
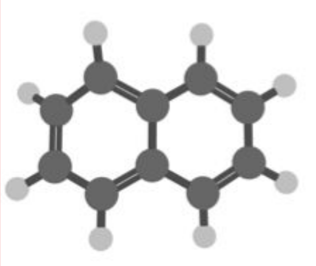
Improving the **safety** dimension of processes

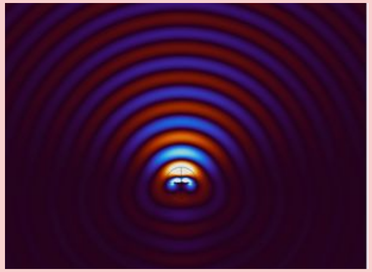
MATERIAL FORMAT: FEM for dust AM simulation



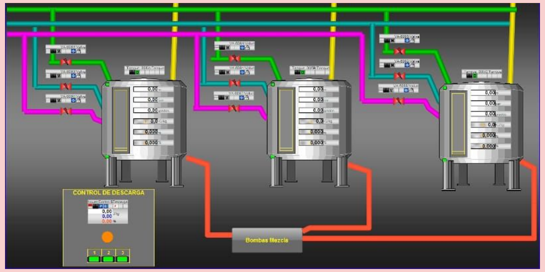
SECONDARY SUBSTANCES: QSAR models



PHYSICAL HAZARDS: FEM for radiation propagation



SAFE ENVIRONMENTS: digital twins of machinery and plant



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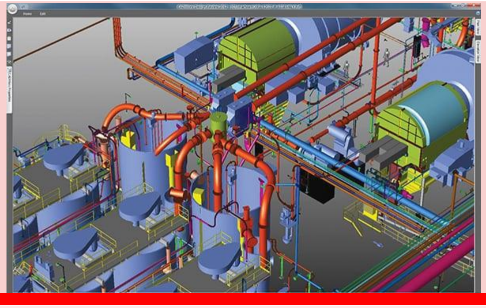
Improving the **sustainability** dimension of processes

MATERIAL EFFICIENCY: AI for zero defect	**ENERGY EFFICIENCY:** digital twin of the whole factory
	
RENEWABLE ENERGY: from fossil fuels to H2, biofuels and electricity	**WHOLE LCA:** reuse, remanufacture, recycle (circularity)
	

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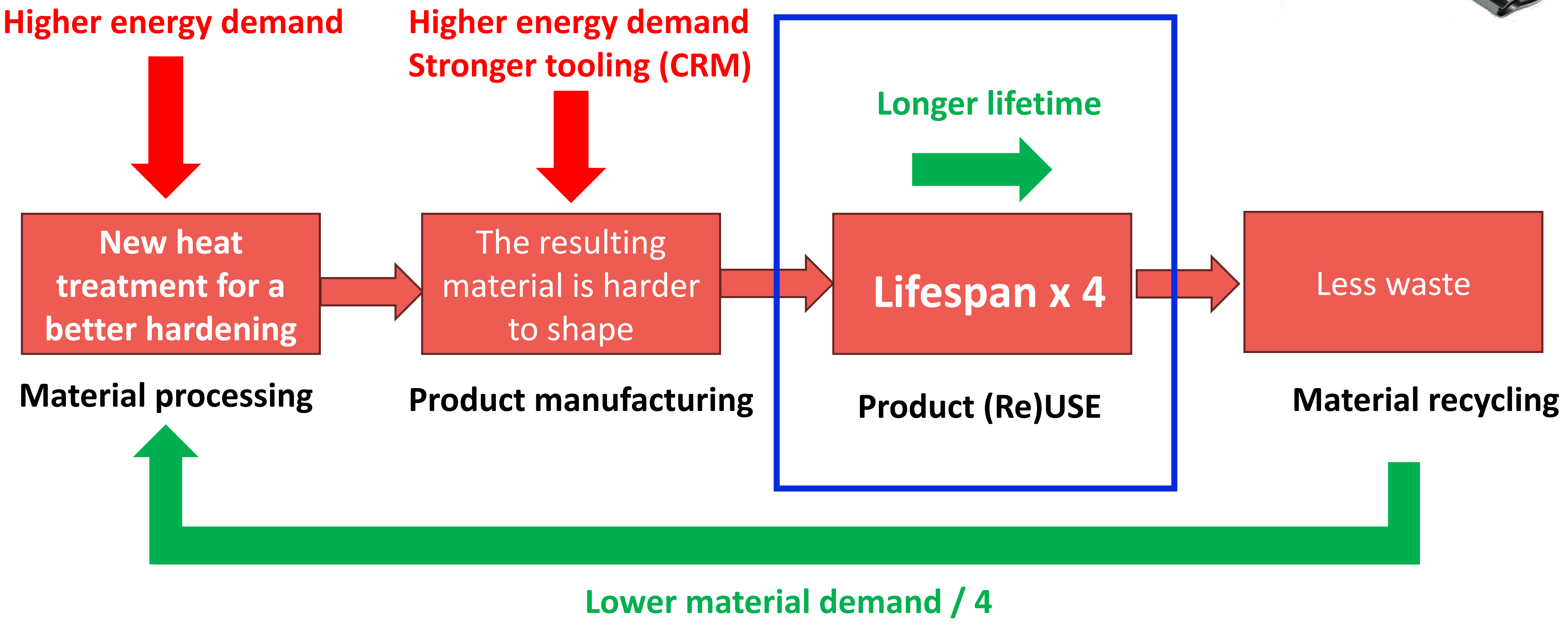
Example: improving the hardness of a **connecting rod material** for a longer lifespan in car **remanufacturing**
Functional unit: 5 000 000 km driven **distance**



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Using the functionality and the performance of materials for the SSbD framework

Francesco Pagano - Tekniker

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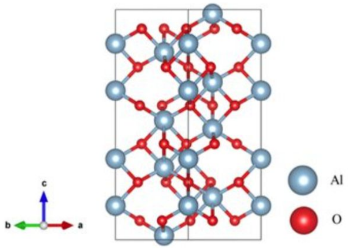
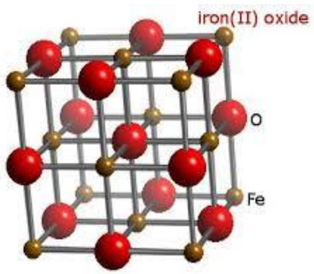
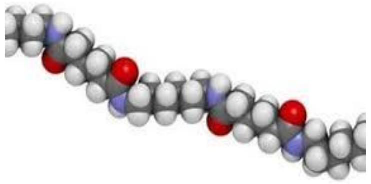
What is a material?







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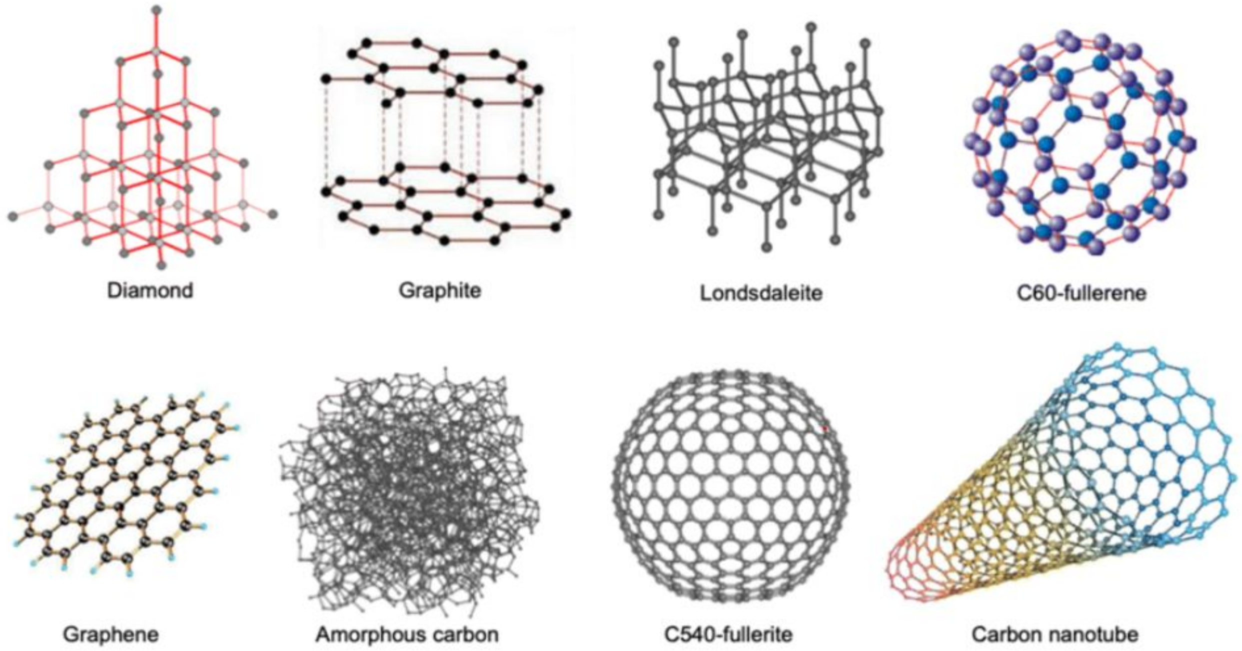
What is a material?



Carbon allotropes: diamond, graphite, lonsdaleite, C60-fullerene, graphene, amorphous carbon, C540-fullerite, and single-walled carbon nanotube

Negri, V., Pacheco-Torres, J., Calle, D. *et al.* Carbon Nanotubes in Biomedicine. *Top Curr Chem (Z)* **378**, 15 (2020). https://doi.org/10.1007/s41061-019-0278-8

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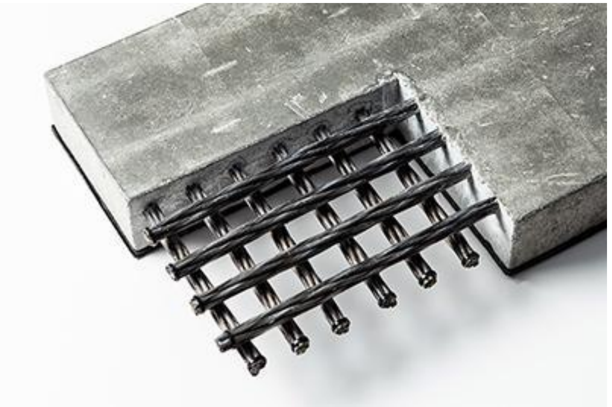
What is a material in the real world?



Impurities
Mixture of chemicals
Structural defects
Inhomogeneous
...

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What determines the properties of the material?

- Microscopic level parameters (atomic composition, crystal structure, bonding type, defects and dislocations, microstructure, phase distribution, etc.)
- Composition (alloying elements, additives, impurities content, etc.)
- Processing (heat treatment, mechanical treatment, ageing, etc.)
- External environment (temperature, pressure, exposure to chemicals, gasses, radiation, etc.)

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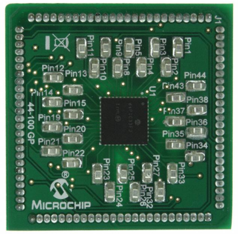

The ability of a material to exhibit specific physical, chemical, mechanical, electrical, optical, or biological properties that make it suitable for a particular purpose

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Anti-stick

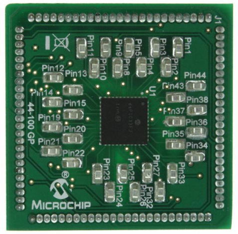
Durable, safe?

Resistant

Warm

UV protection

Fast?



Biocompatibility?

Colored?

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Anti-stick, anti scratch, thermal resistant, thermal conductive, etc.

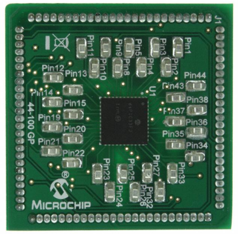
Durable, resistant to puncture, high coefficient of friction, etc.

High tensile strength, flexibility, light, etc.

Thermal insulation, durable, waterproof, breathability, etc.

UV protection, spreadability, water resistance, etc.

Semiconducting behavior, electrical conductivity, dielectric constant, etc.



Biocompatibility, osteointegration, low wear, low friction, etc.

Water resistant, UV resistant, corrosion resistant, etc.

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The material is part of a system and should be considered in the context and in the environment of use

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What is the purpose of the material?

Can I modify the material to be more sustainable and still functional?

Are there alternative solutions with the same functionality?

Are there secondary properties that should be taken into account?

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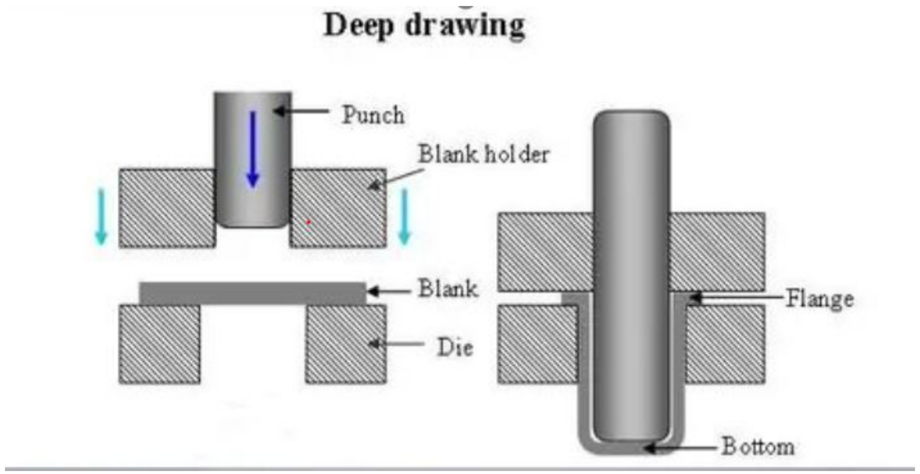

Requirements for deep drawing process

- Low friction between the die and the workpiece.
- Protects tooling from adhesive and abrasive wear.
- Withstands high temperatures generated during rapid forming without degradation or breakdown.
- ...

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Material to be substituted: Chlorinated paraffines, a toxic component of the lubricant that provides good lubricity and wear resistance.

Options:

- To maintain the formulation and substitute only the "problematic" component
- To find a new formulation alternative to the previous one.
- <u>To adopt a completely new solution that can have the same functionality of the lubricant (e.g. coating)</u>

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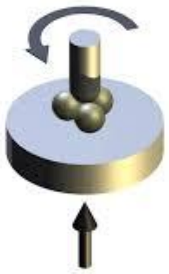
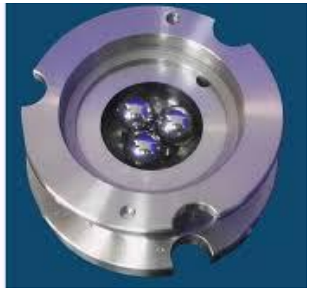
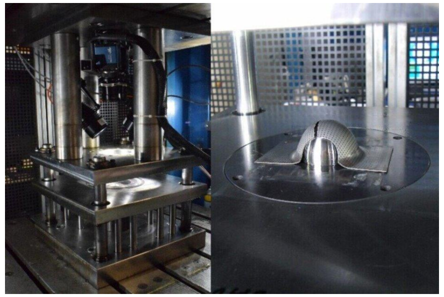
Laboratory tests to compare the different alternatives







Name			
Solution	Coefficient of friction	Wear	Thermal stability
Reference	0.12	0.6 mm	230
Alternative oil	0.12	0.7 mm	215
Coating	0.12	0.6 mm	400

The coating improve the properties that were attributed to the chlorinated paraffine hence it can be adopted as alternative solution!!!

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Failure of the solution because the coating do not provide heat dissipation.

LESSON LEARNED: **it is possible to replace a material with a different solution**, but it necessary to analyse thoroughly the functionality that need to be replaced.

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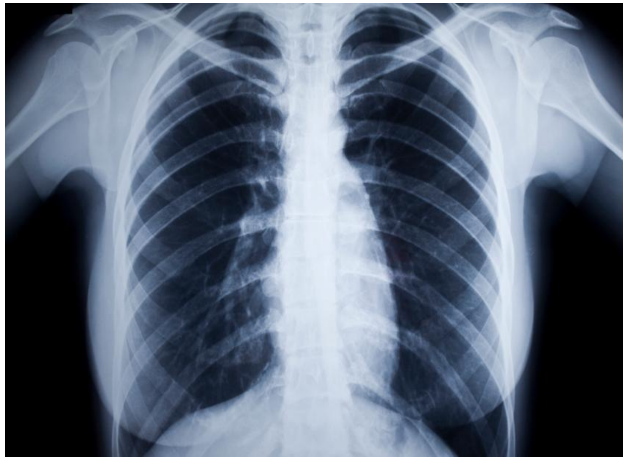
- **Temperature** (high temperature, low temperature, thermal cycling, etc.)
- **Chemical environment** (exposure to acids, bases, electrolytes, gases, etc.)
- **Atmospheric Pressure** (vacuum conditions, high pressure)
- **Biological Exposure** (microbial attack, biofouling)
- **Radiation** (Solar, UV, X-Rays, etc.)
- **Mechanical loading conditions** (contact pressure, load, dynamic load, vibrations, etc)



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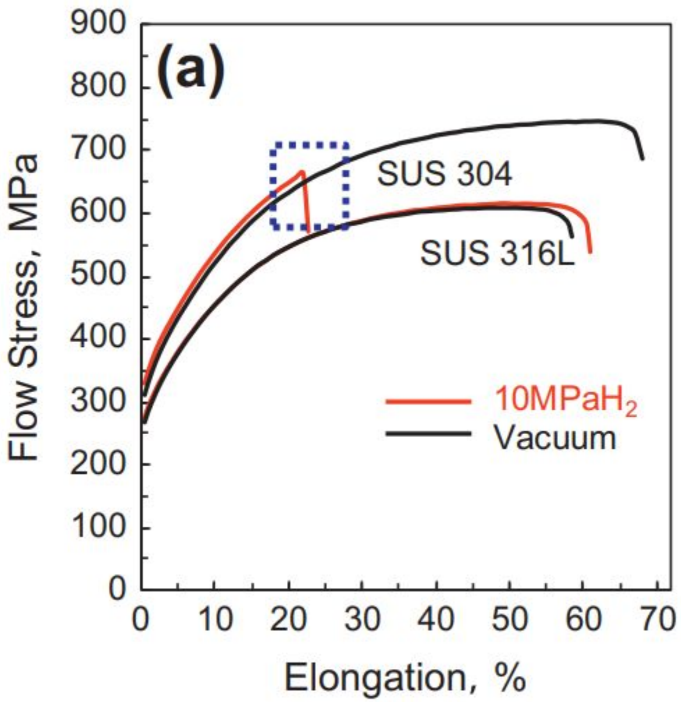
Hydrogen embrittlement



Acta Materialia, 67(),
342-353. doi:10.1016/j.actamat.2013.12.039

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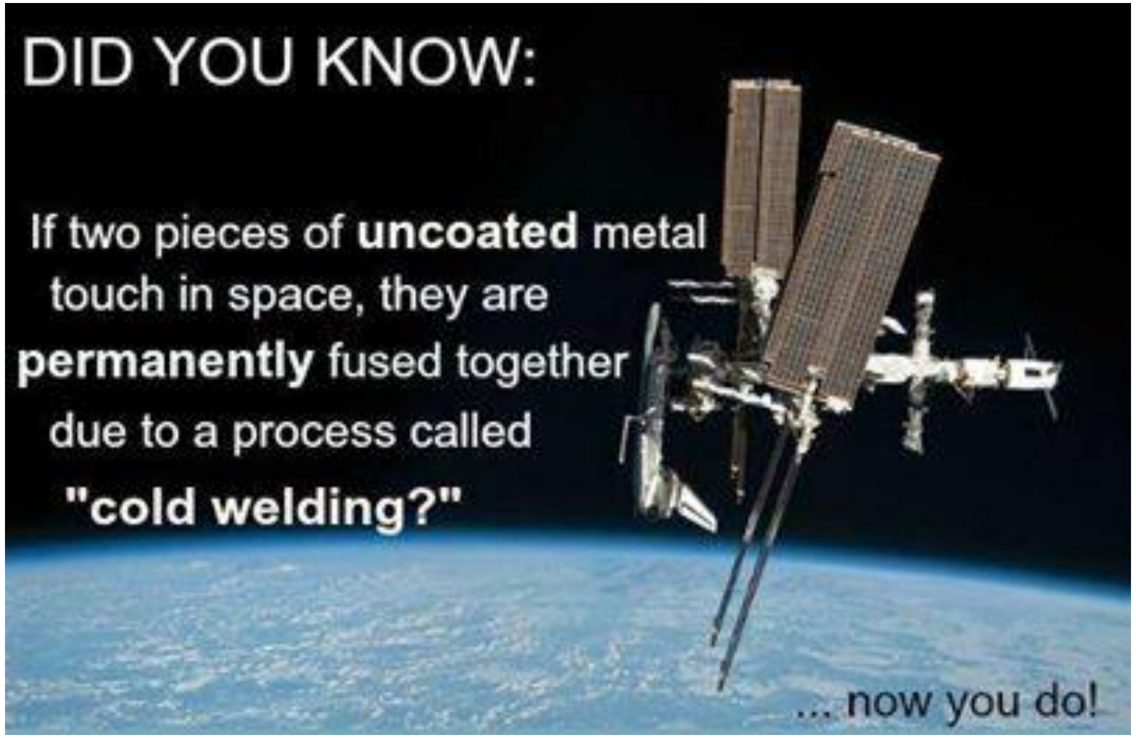
Why Metals Spontaneously Fuse Together In Space

https://www.youtube.com/watch?v=Y2nQ8isf55s



Not always an obvious path to the functionality

Anti-icing functionality

- Contact angle
- Ice adhesion strength
- Freezing time

If there are not valid standards, robust testing methods need to be developed

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The requirements of the application are essential to differentiate between critical, optional or useless properties

Paint for steel bridge

Corrosion resistance	Critical
Adhesion to steel	
Water resistant	
UV resistance	
Colour Retention	Optional
Stain resistant	
VOC content	
Food grade safety	Useless
Soft touch finish	

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Paint for steel bridge

We need a testing method and evaluation criteria to define if the material is suitable for a given application. It is posible to define performance limits.

Property	Category	Standard Test	Acceptable Value / Criteria
Adhesion to metal	Critical	ASTM D3359 (Cross-cut tape test)	Classification 4B or 5B (minimal/no paint removal)
Corrosion resistance	Critical	ASTM B117 (Salt spray test)	No rust, blistering, or delamination after 1,000+ hours
UV resistance	Critical	ASTM G154 (QUV accelerated aging)	ΔE (color change) < 5 after 500–1,000 hours
Water resistance	Critical	ASTM D870 (Water immersion)	No blistering, peeling, or softening after 24–96 hours
Color retention	Optional	ASTM D2244 (Color change by ΔE)	ΔE < 3 (for architectural-grade appearance)
Graffiti resistance	Optional	ASTM D6578/D6578M	Class 1–2 (easy removal of graffiti agents)
Low VOC content	Optional	ASTM D3960 / EPA Method 24	< 250 g/L (VOC content for industrial coatings)
Transparency	Useless	ASTM D2805 (Hiding power)	Not applicable — full opacity is desired
Food-grade safety	Useless	FDA 21 CFR 175 (only for food-contact)	Not applicable for the use case
Soft-touch finish	Useless	Tactile feel (subjective or custom)	Not needed for the use case

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Paint for steel bridge

Property	Solution 1	Solution 2	Solution 3
Adhesion to metal	4	5	3
Corrosion resistance	3	5	1
UV resistance	2	4	2
Water resistance	1	0	2
Color retention	4	3	4
Graffiti resistance	2	4	5
Low VOC content	1	0	4
Transparency	3	2	4
Food-grade safety	0	2	4
Soft-touch finish	3	4	5
Scale 1 to 5 (0 means below acceptable limit)			

If the material does not meet the minimum required performance, it cannot be considered suitable for the application. It is possible to give define the leading parameters for the selection of the best candidate or to calculate a weighted average by assigning varying degrees of importance to each parameter.

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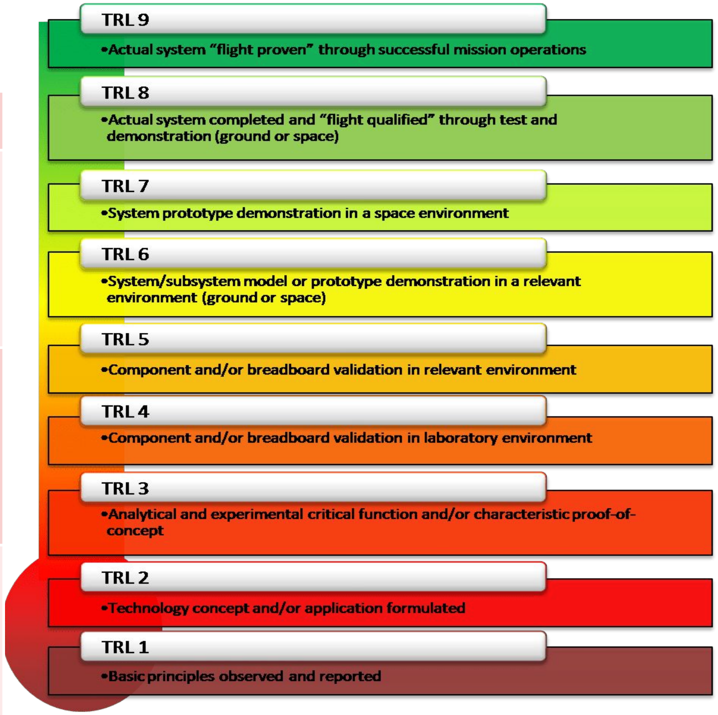
Technology Readiness Level for characterization (NASA)

TRL	Stage	Goal of Characterization	Techniques Used
1–3	Discovery & fundamental research	Understand intrinsic properties (structure, composition, basic performance)	XRD, TEM/SEM, FTIR, UV-Vis, TGA, DSC, XPS
4–6	Lab-scale validation & optimization	Evaluate processability, repeatability, stability, integration with prototypes	Rheology, mechanical testing, electrical tests, accelerated aging
7–9	Pre-commercial & deployment	Ensure reliability, durability, compliance, and scalability	In-situ/real-time testing, long-term stability studies, environmental testing standardization



https://www.nasa.gov/directorates/somd/space-communications-navigation-program/technology-readiness-levels/

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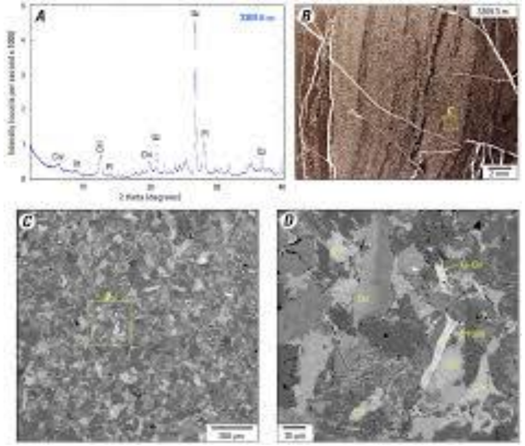
Low Technology Readiness Level (1-3)

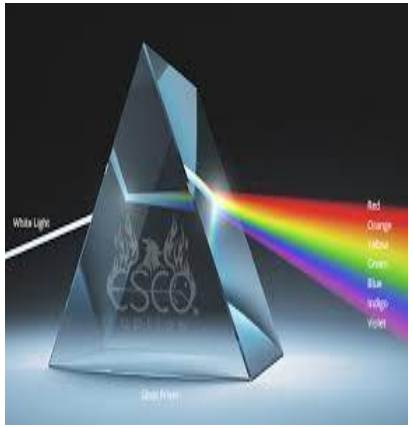
Objective: Understand intrinsic properties (structure, composition, basic performance)

Structure/Morphology



Chemical composition

Physical/chemical properties



Mechanical properties

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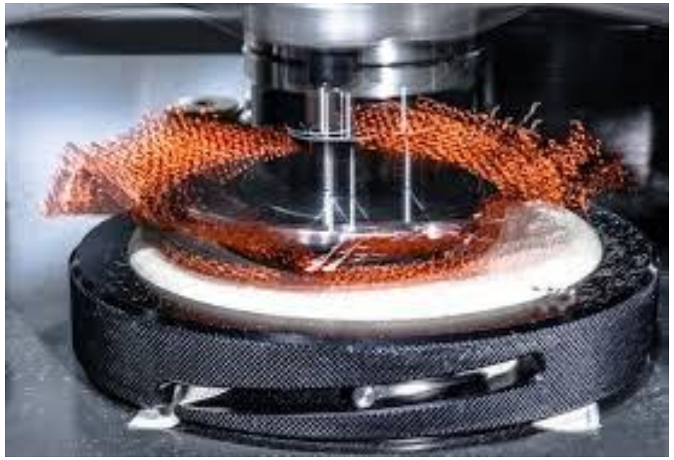
Mid Technology Readiness Level (4-6)

Objective: Evaluate processability, repeatability, stability, integration with prototypes



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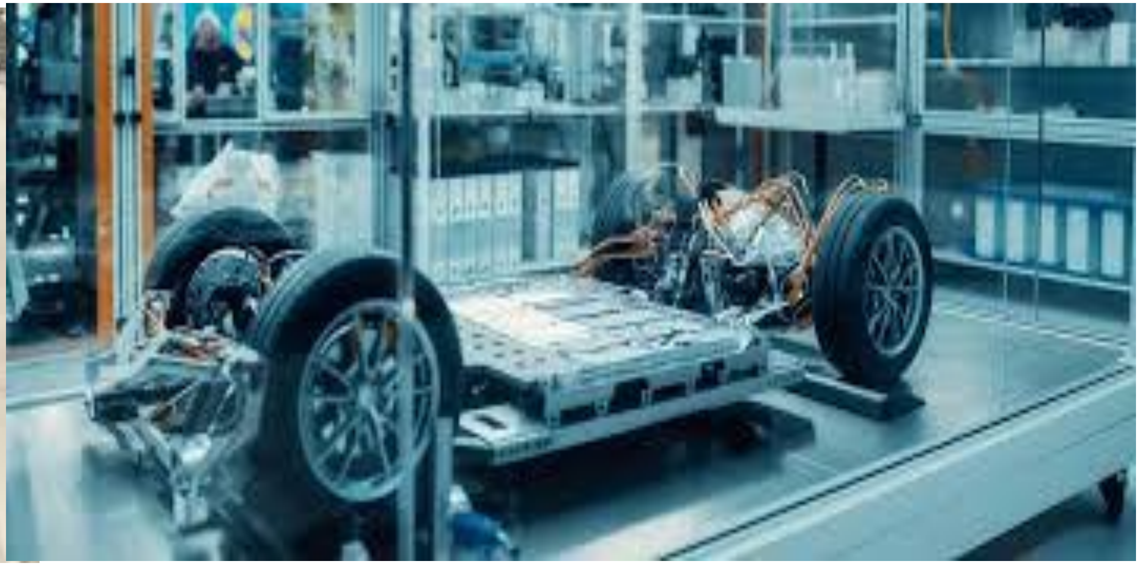
Low Technology Readiness Level (7-9)

Objective: Ensure reliability, durability, compliance, and scalability



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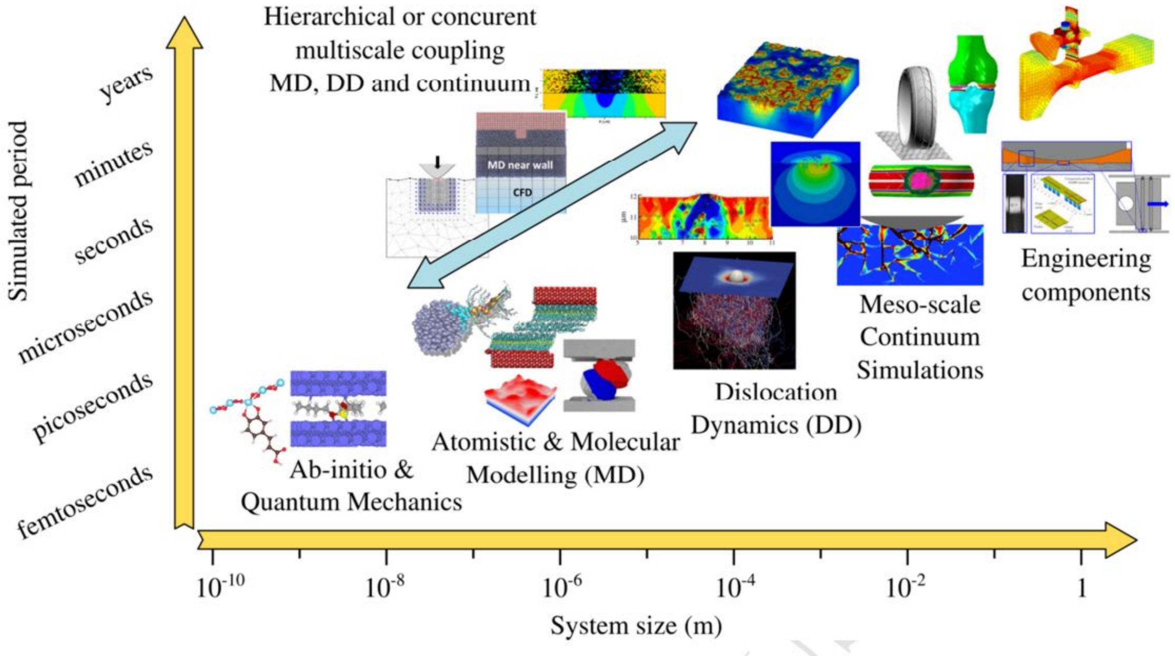
Multidimensional modelling

Early TRL (1–3):
- Ab Initio / First-Principles Modeling
- Molecular Dynamics

Mid TRL (4–6):
- Meso-scale Continuum Simulation
- FEM

High TRL (7–9):
- Engineering models
- Multiphysics Modeling
- Machine learning and data driven



https://www.sciencedirect.com/science/article/abs/pii/S0301679X18300756

TRL Range	Modeling Type	Scale	Modeling Goal	Characterization Needs
1–3	Ab initio, Molecular Dynamics,	Atomic	Understand intrinsic material behavior	- **Crystallography** (XRD, TEM)- **Spectroscopy** (FTIR, Raman, XPS)- **Thermal Analysis** (DSC, TGA)- **Density, porosity**- **Elemental analysis** (EDX, ICP)
3–5	Mesoscale, Micromechanic	Micro / Meso	Predict microstructure-pro perty links	- **Microstructural analysis** (SEM, EBSD, AFM)- **Mechanical testing** (nanoindentation, microtensile)- **Phase identification**, grain size distribution- **In-situ microscopy**
5–7	Finite Element Analysis, Continuum Models	Meso / Macro	Simulate structural and environmental response	- **Mechanical performance** (tensile, fatigue, creep)- **Thermal and environmental stability**- **Non-destructive testing** (NDT, CT scans)- **Dimensional inspection** (CMM, laser scanning)
7–9	Multiphysics, Reduced-order, Data-driven	Macro / System	Predict and monitor real-world performance	- **Full-scale component testing**- **Field data acquisition** (strain gauges, thermocouples)- **Accelerated aging tests**- **System-level validation** (vibration, corrosion, weathering)- **Digital twin feedback**

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Example of case study: Lubricant for offshore wind turbine

It is needed to use safe and biodegradable lubricants because of the risk to have oil spillage in the water

Role of the lubricant:

- Reduction of friction
- Extension of the life of the gear box components
- …

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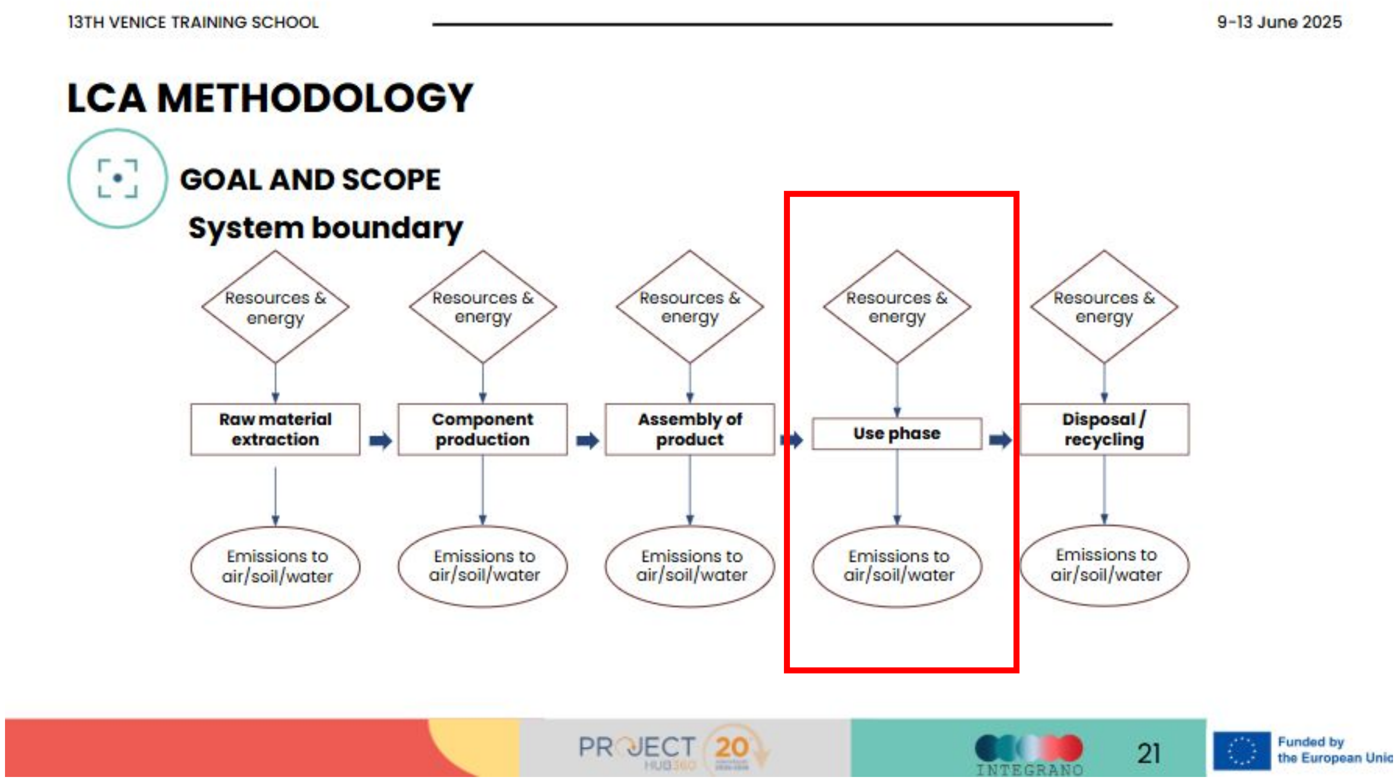
Example of case study: Lubricant for offshore wind turbine



Introduction to Life Cycle Assessment. Mattia Costamagna

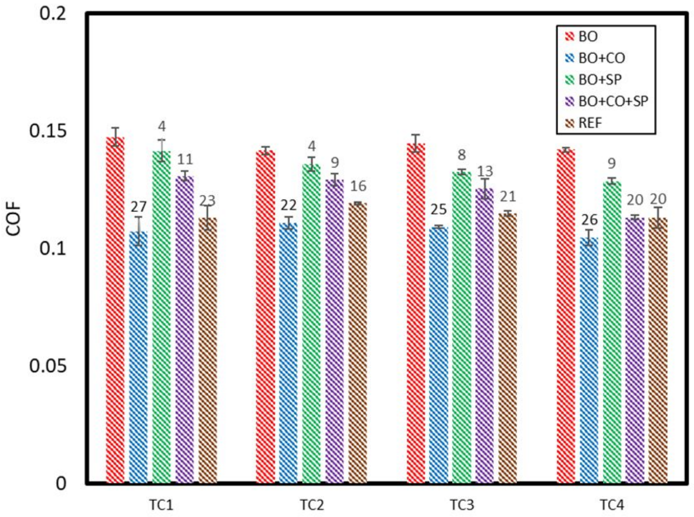
Resources and energy:

Friction reduction --> energy saving

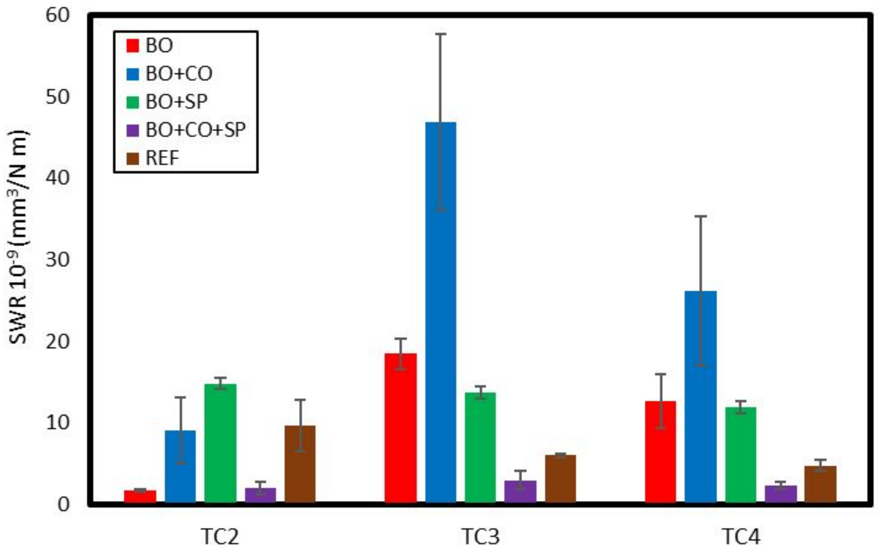
Extended component life --> Energy saving

Example of case study: Lubricant for offshore wind turbine

Can we estimate the energy savings?



Coefficient of friction



Wear

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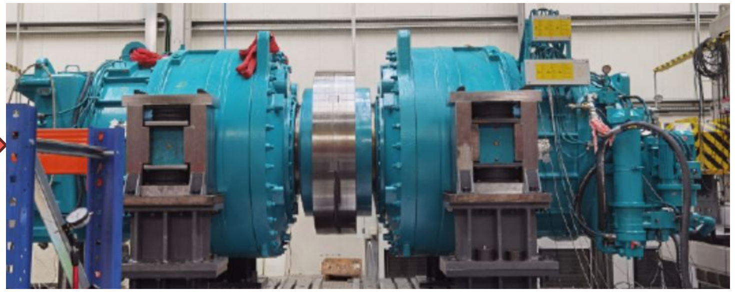
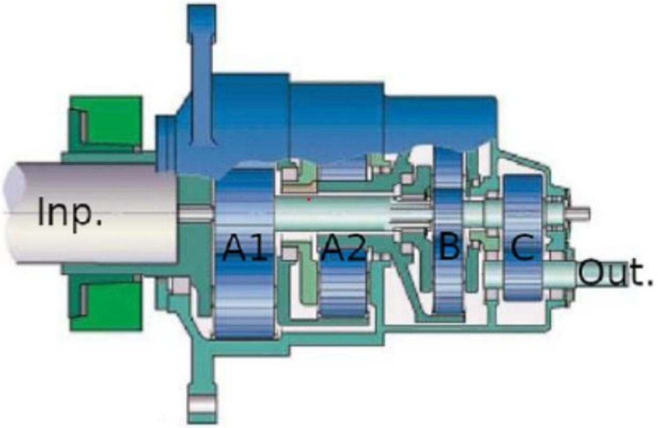
Example of case study: Lubricant for offshore wind turbine

TRL3-4

TRL5-6

TRL?





Power loss in rolling bearings and gears lubricated with wind turbine gear oils.
DOI: 10.13140/RG.2.1.5007.4083

Testing and modelling of a 2.5 MW wind turbine gearbox: Influence of lubricant formulation.
https://doi.org/10.1007/s10010-023-00716-0

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Example of case study: Sunscreen

Main function: UV Protection

Secondary functionality that could have an impact on the safety and sustainability:

- Photostability
- Water and Sweat Resistance
- Stability and Shelf-Life

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Example of case study: Textiles

Main function: Comfort and durability

Secondary functionality that could have an impact on the safety and sustainability:

- Tensile Strength
- Abrasion Resistance
- Ageing

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https://sitolub.eu/

ALCHEMISSTS

Funded by the European Union under the Grant Agreement No. 101178074.

https://www.alchemissts-project.eu/

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Swiss Confederation

Federal Department of Economic Affairs, Education and Research EAER
State Secretariat for Education, Research and Innovation SERI

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