



SiTOLub

*SIMULATION TOOLS FOR
THE DESIGN OF SAFE AND
SUSTAINABLE LUBRICANTS*

4.04.T02 – A Fully Automated Life Cycle Assessment Model for SSbD-Driven and Circularity-Oriented Lubricant Design

20/10/2026

SETAC Europe 27th LCA Symposium

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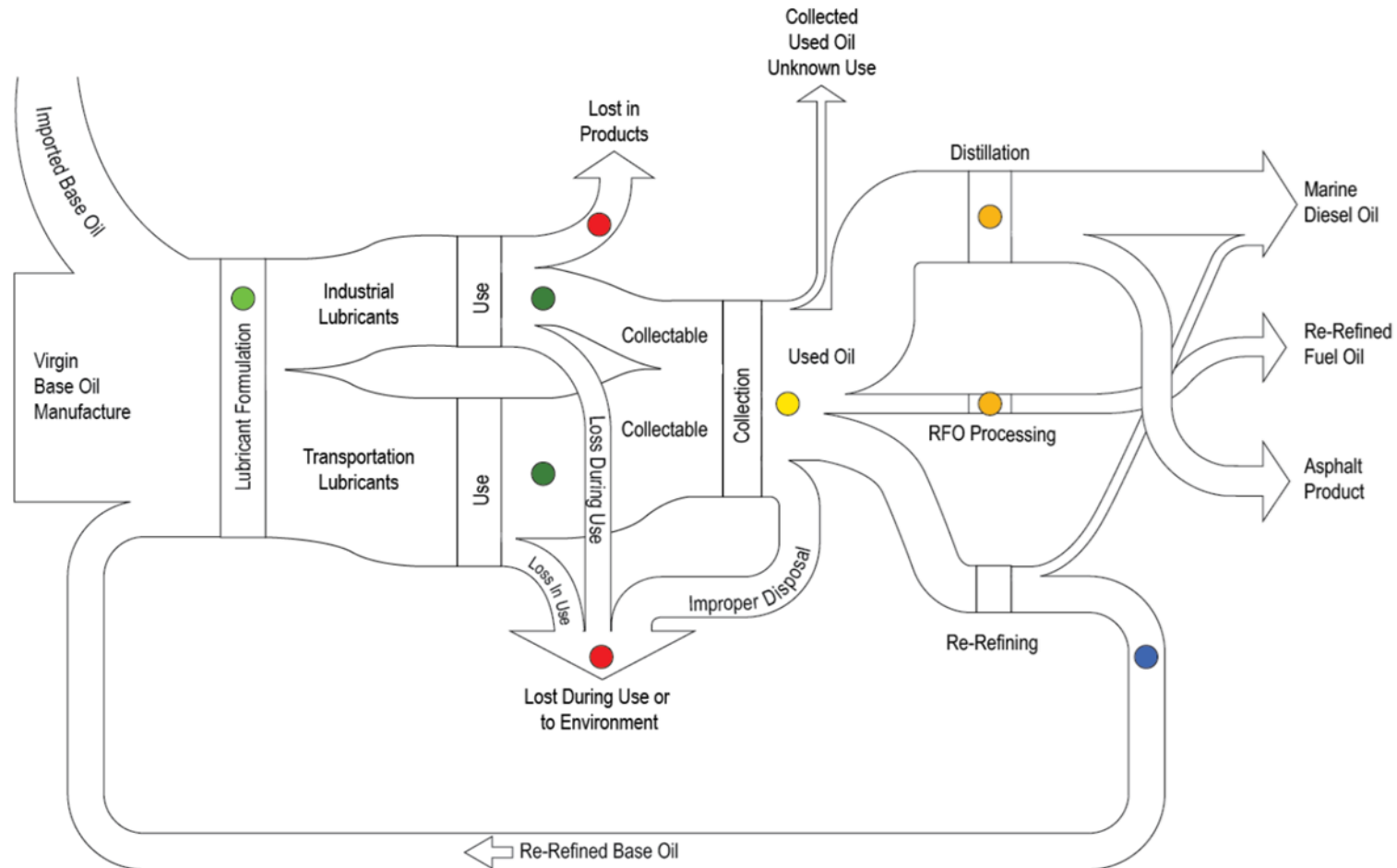
GreenDelta

Introduction

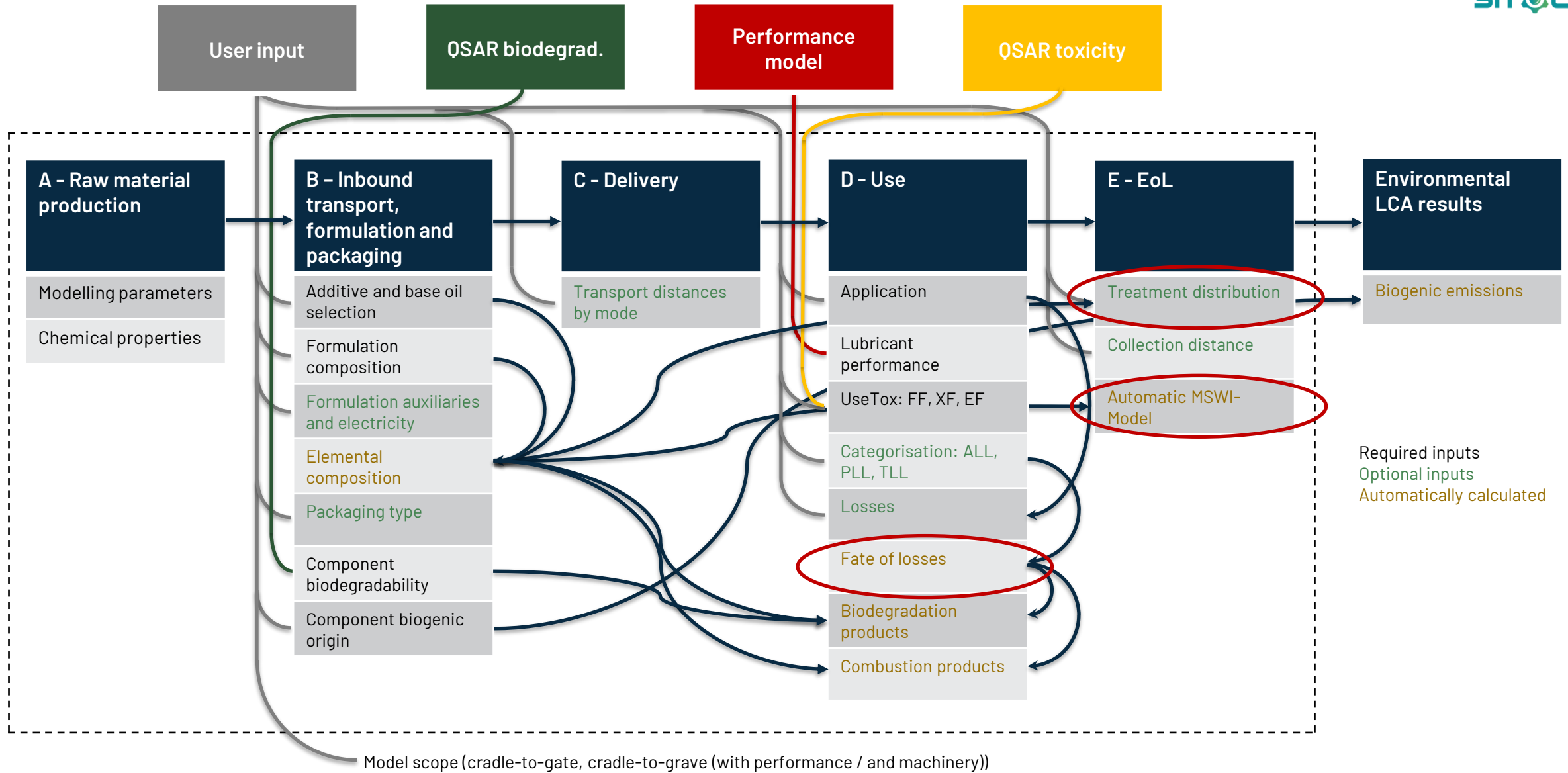
- **Lubrication enables key mechanical processes** that keep the economy running smoothly
 - **SiToLub**: Research project focused on **improving lubrication chemistry**
 - While lubrication may reduce overall environmental impact of processes, **involved chemicals are critical → environmental release** could occur
- Development of a **virtual platform** integrating computational models from a variety of fields
- Prediction of **performance, toxicity, sustainability implications**
 - As part of the environmental LCA: **flexible modelling approach dependent on lubricant formulation and application** to estimate fate along the life cycle

SSbD6 – Reduce exposure to hazardous substances	SSbD7 – Design for end-of-life
SSbD8 – Consider the whole life cycle	SSbD9 – Ensure responsible sourcing and minimise social risks

The Lubricant Life Cycle

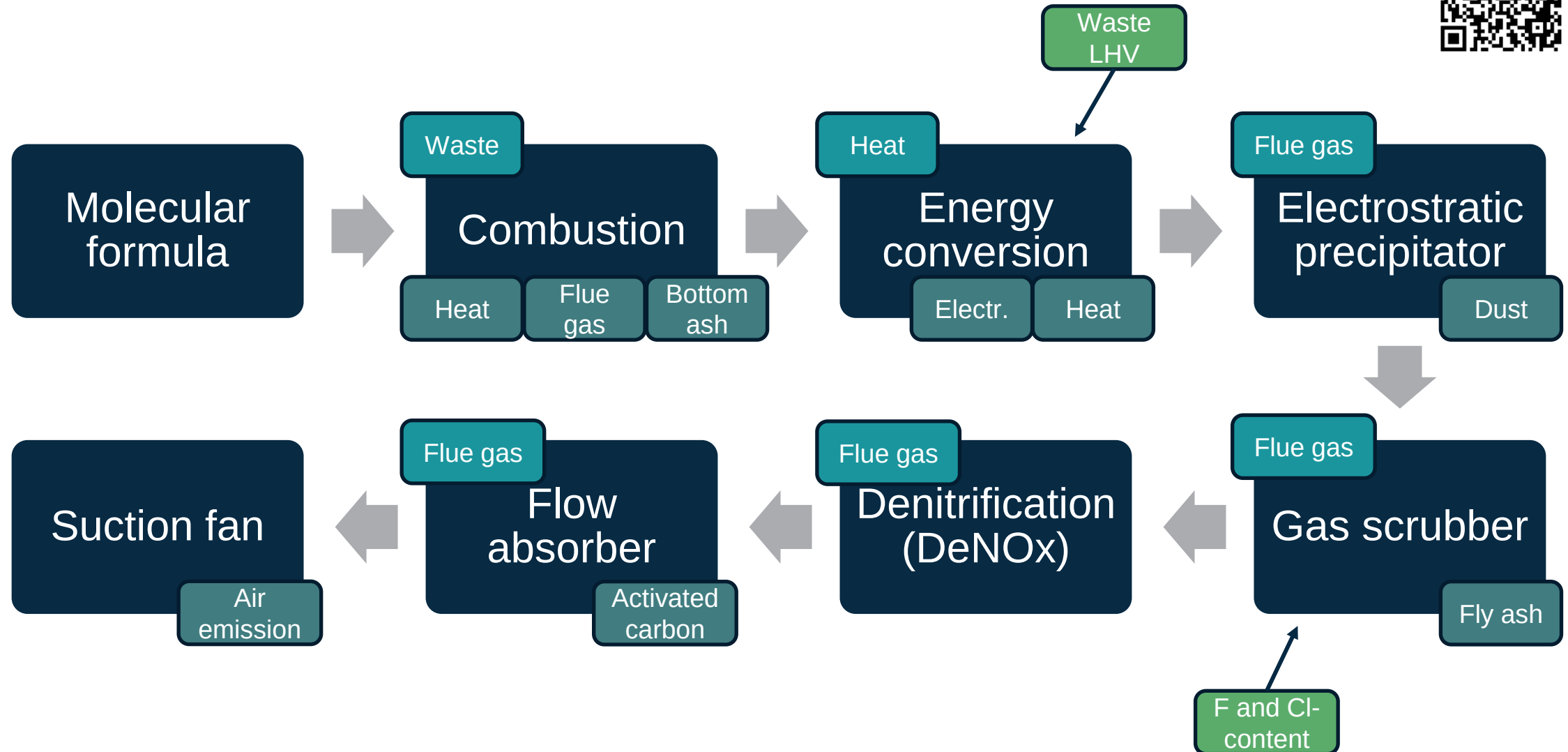


US Department of Energy: Used Oil Management and Beneficial Reuse Options to Address Section 1: Energy Savings from Lubricating Oil Public Law 115-345.

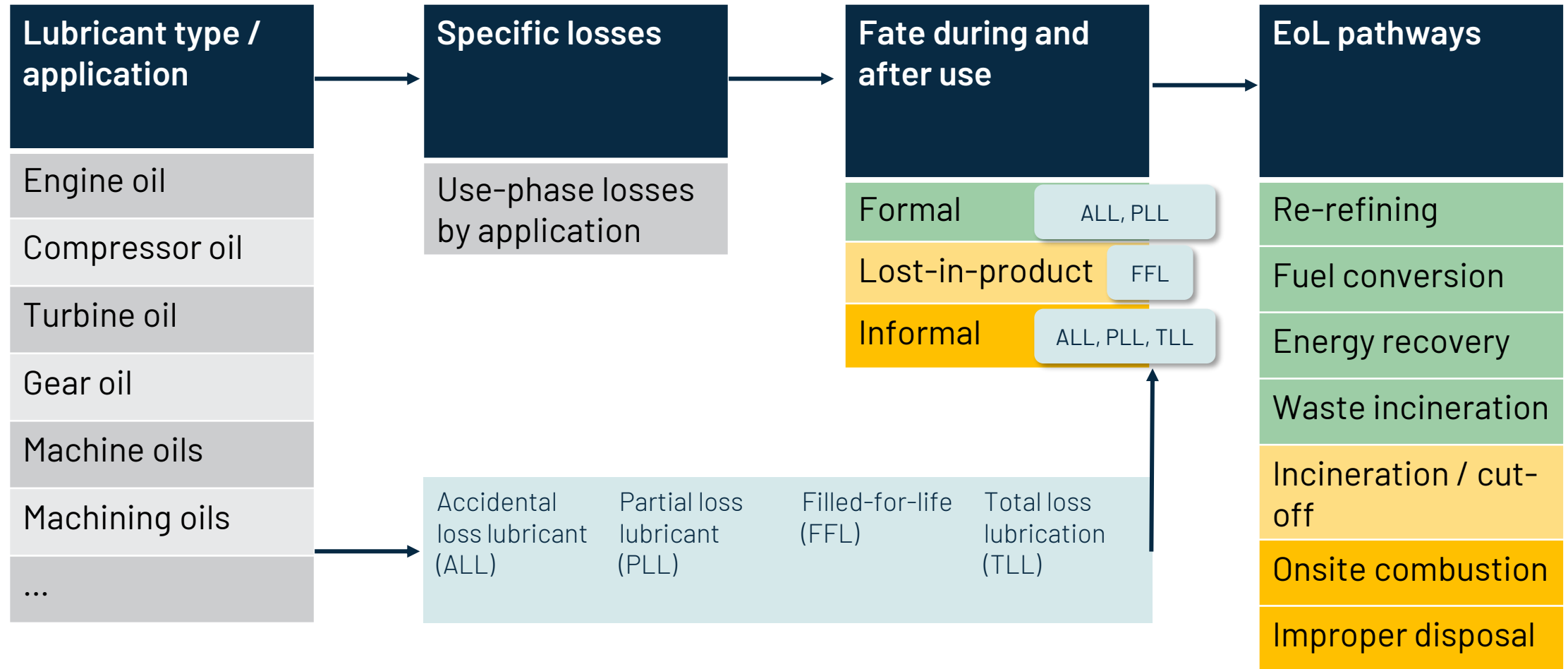




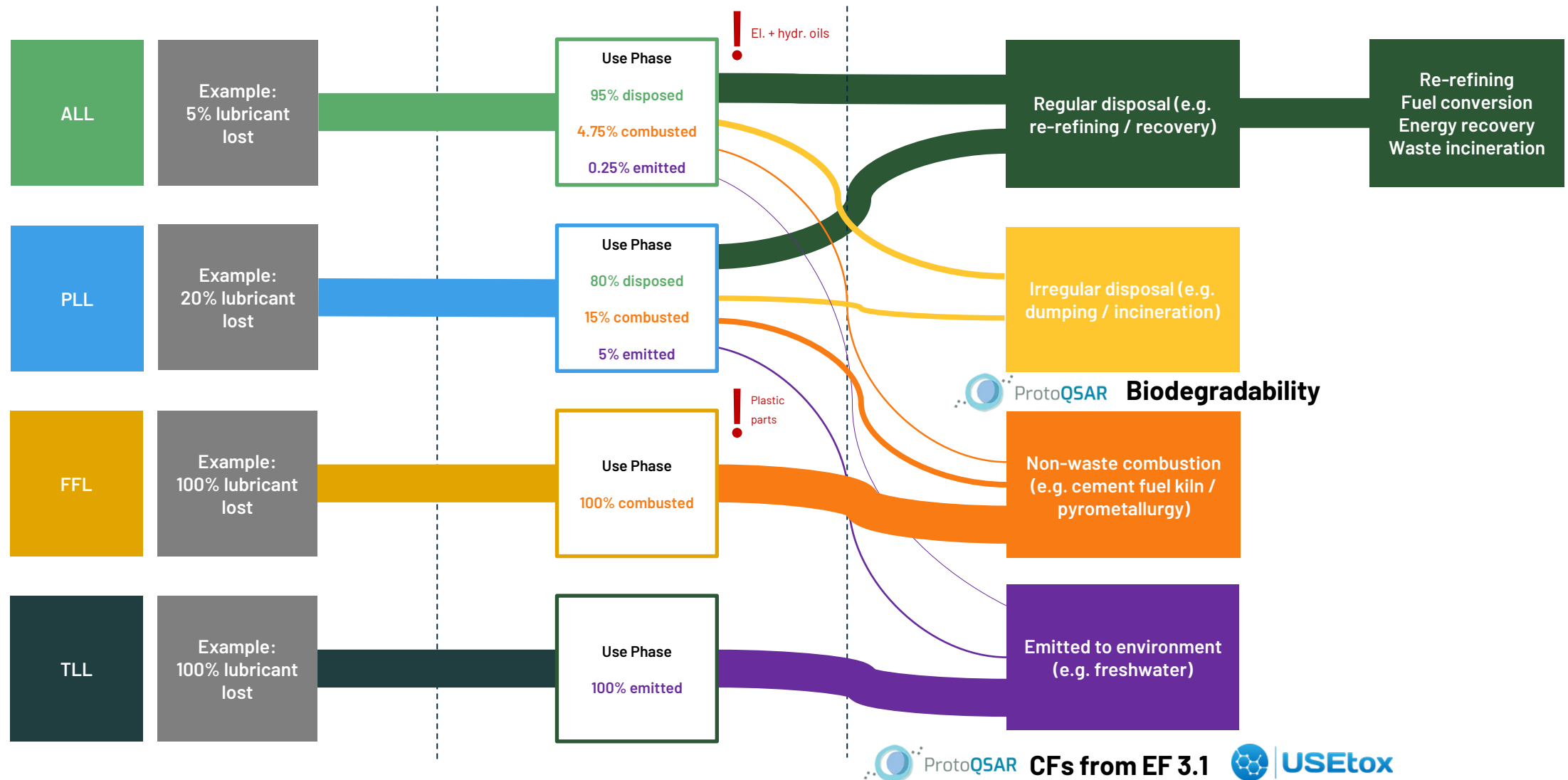
Automatic municipal solid waste incineration



Application-specific EoL modelling



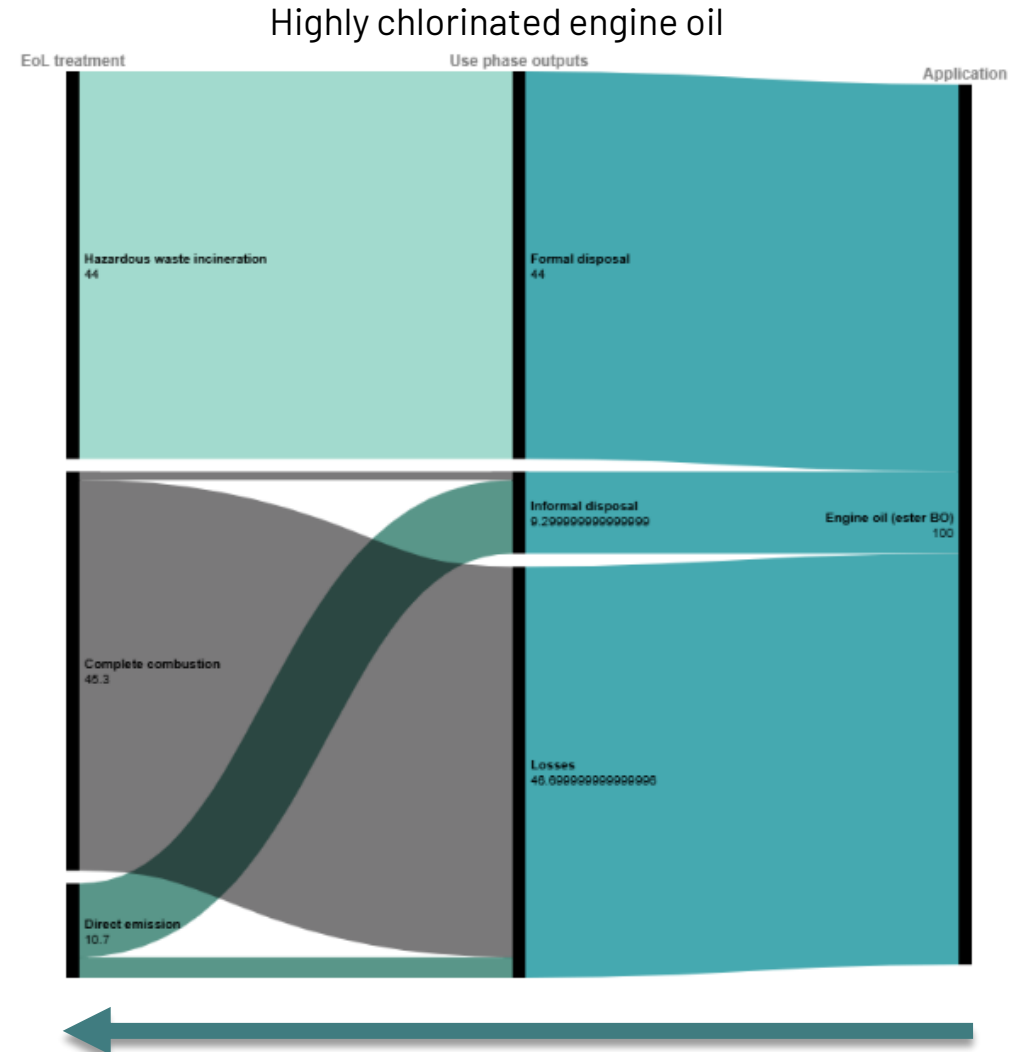
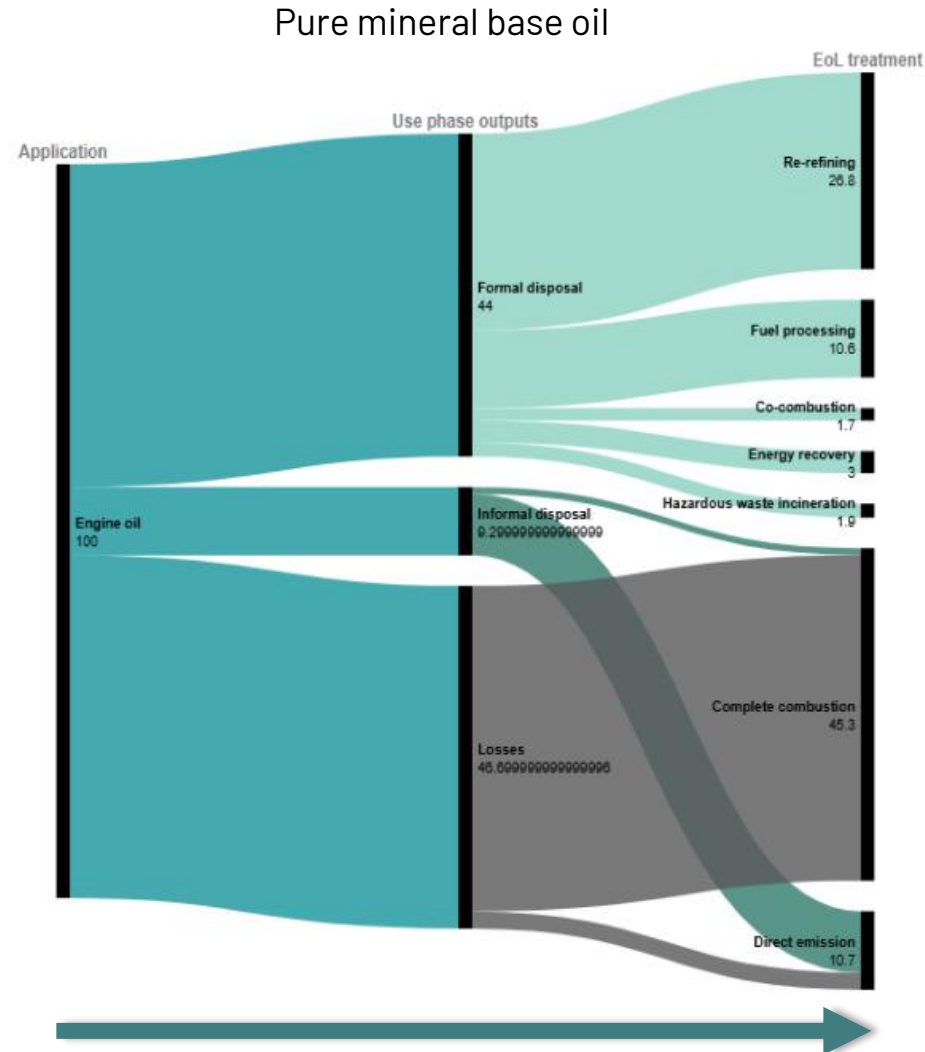
Simplified fate of losses in use



Chemistry determines feasible EoL pathway

Formulation constituents	Threshold	Effect (reasoning)
Chlorine (Cl)	500 ppm / 2000 ppm	No re-refining / incineration (interaction with catalyst)
Esters	>3% ester content	No re-refining (downcycling to fuels)
Silicon (Si)	>5% silicone content	No re-refining (interaction with catalyst)
Glycols	>1% glycol content	No re-refining (interaction with catalyst)

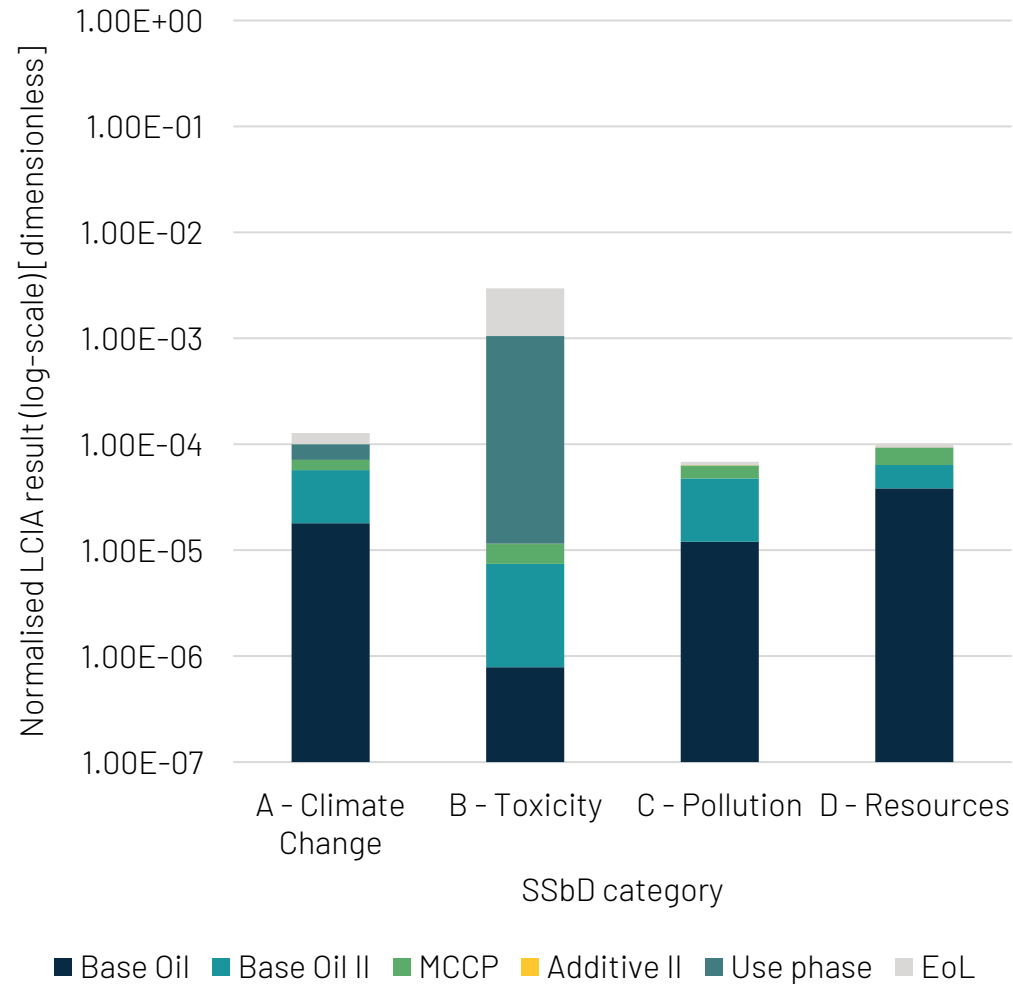
Exemplary fate of potential formulations



How to derive design recommendations?

Use case (application)	Loss category	Biogenic origin	Waste or recycled source	Low toxicity additives	Model end-of- life fate	Key design and SSbD
Metal working additive	ALL					

LCA for one compound – MCCP formulation



- **Metalworking fluid** application, **ALL** classification
- **Toxic additives** have a direct and **visible impact** in the model
- **Emissions in the use phase** and at the **end of life** dominate toxicity impacts
- Production impacts roughly **equivalent to mass share** in formulation
 - Exception: biogenic **second base oil**

Design recommendations

Use case (application)	Loss category	Biogenic origin	Waste or recycled source	Low toxicity additives	Model end-of-life fate	Key design and SSbD
Base oil (engine oil)	ALL	✗	✓	✓	Recycling (re-refining)	Recyclable (SSbD 7 + 8)
Solid anti-wear additive (grease)	FFL	✓	✓	✗	Incineration (0 recovery)	MSWI compatible (SSbD 7 + 8)
Metal working additive	ALL	✓	✓	✓	Combustion (largely during use)	MSWI compatible (SSbD 7 + 8)
Corrosion inhibitor (pipe dope)	TLL	✓	✓	✓	Total loss (full emission)	Biodegradable (SSbD 6 + 8)

Conclusions

- SSbD requires consideration of the **whole life cycle**
 - **Prospective downstream fate** of the product needs to be assessed **at an early design stage**
- **Prediction of end of life fates for lubricants** can be achieved based on:
 - Specific lubricant formulation
 - Application and classification of the lubricant
- The fate of the formulation as a whole is **highly dependent on the application and formulation** of the lubricant
 - Remaining collectable lubricant fraction
 - Re-refining compatibility
- Design **recommendations need to account for lubricant specifics**, especially application and classification of the lubricant

Thank you!

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Acknowledgements

- The *SiToLub* project has received funding from the European Union through the European Health and Digital Executive Agency (HADEA) under grant agreement number 101138807.
- The authors sincerely acknowledge this support and thank all consortium members and collaborators involved in the project.