LCM 2025

1262

SIMULATION TOOLS FOR THE DESIGN OF SAFE AND SUSTAINABLE LUBRICANTS

Integrating Risk, Performance, and Sustainability: Life-Cycle Assessment as a Cornerstone for Safe and Sustainable by Design Lubricants

GreenDeLTa

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openLca

LCM 2025, Palermo

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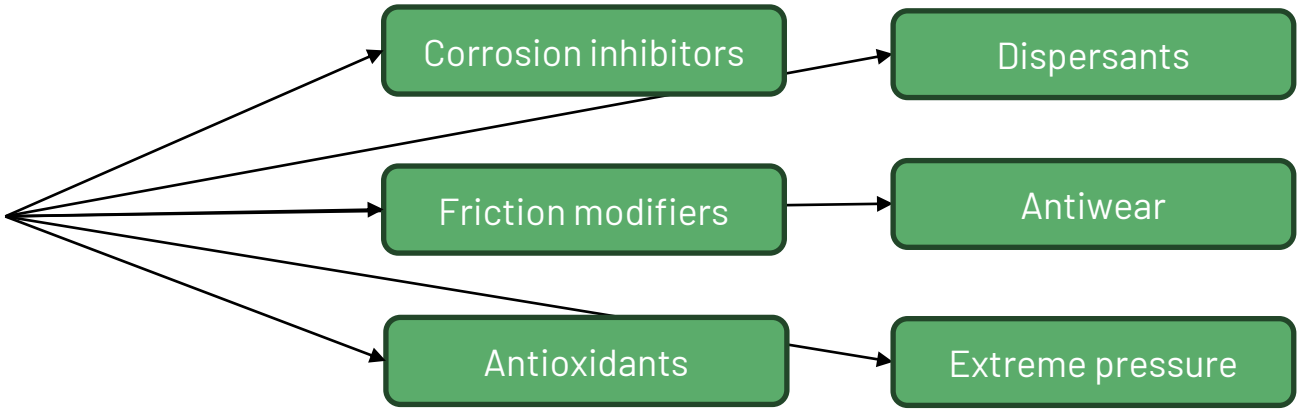
COMPONENTS OF LUBRICANTS

API BASE OIL CATEGORIES					
	Base Oil Category	Sulfur (%)		Saturates (%)	Viscosity Index
Mineral	Group I (solvent refined)	>0.03	and/or	<90	80 to 120
Mineral	Group II (hydrotreated)	<0.03	and	>90	80 to 120
Mineral	Group III (hydrocracked)	<0.03	and	>90	>120
Synthetic	Group IV	PAO Synthetic Lubricants			
Synthetic	Group V	All other base oils not included in Groups I, II, III or IV			



What industry is facing:

What costumers want:

Industry is in need for novel safe and sustainable solutions!

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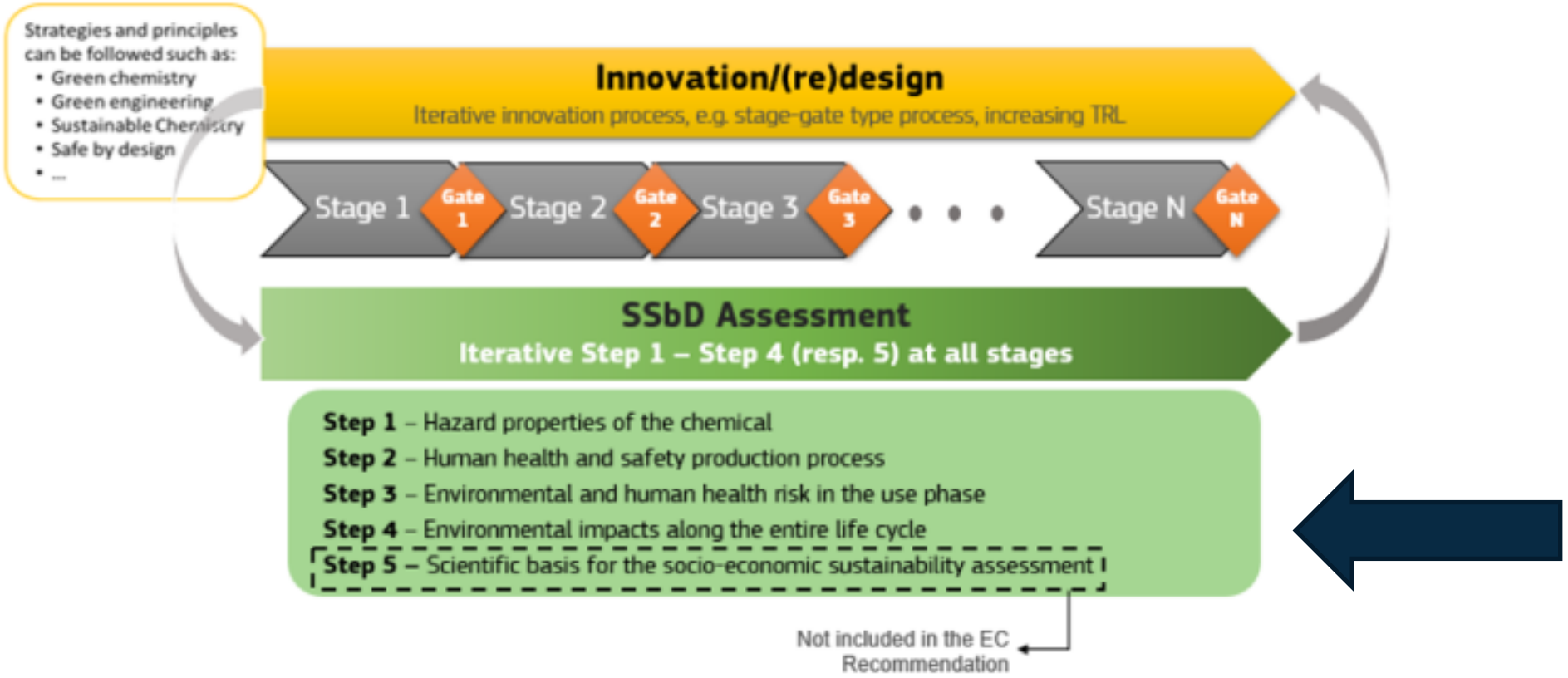
SSbD Framework – Innovating Safe and Sustainable



Caldeira, C., Garmendia Aguirre, I., Tosches, D., Mancini, L., Abbate, E., Farcal, R., Lipsa, D., Rasmussen, K., Rauscher, H., Riego Sintes, J. and Sala, S., Safe and Sustainable by Design chemicals and materials - Application of the SSbD framework to case studies, Publications Office of the European Union, Luxembourg, 2023, doi:10.2760/329423, JRC131878.

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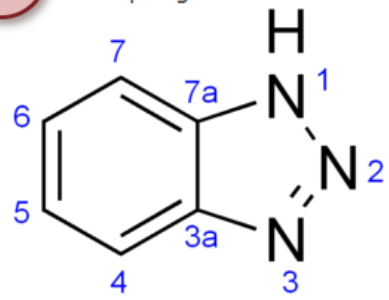
WORKING FLOW

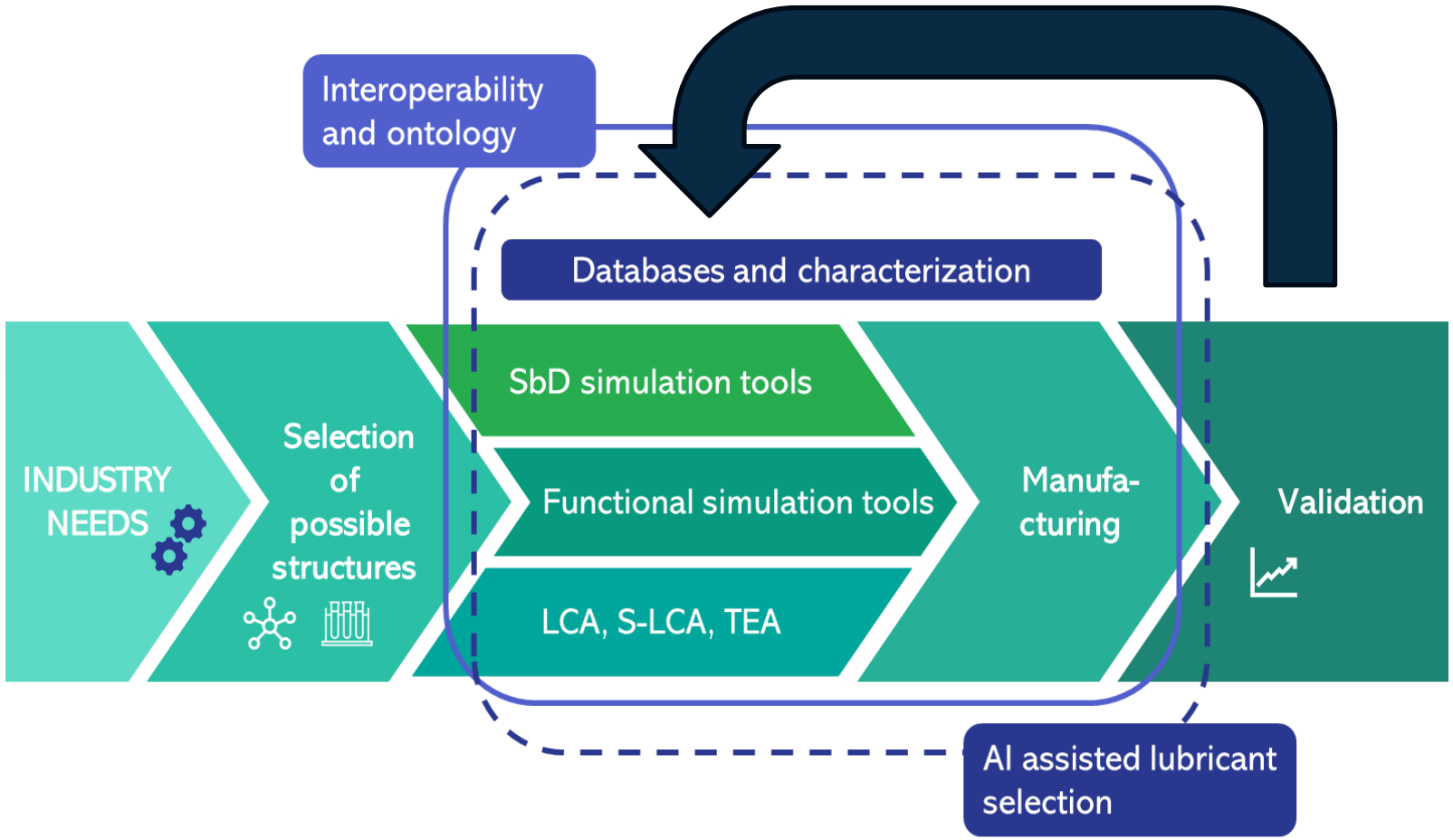
Properties of concern

PBT — Under assessment as Persistent, Bioaccumulative and Toxic

ED — Under assessment as Endocrine Disrupting



benzotriazole



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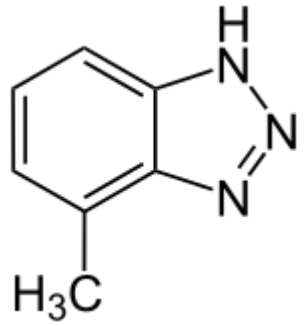
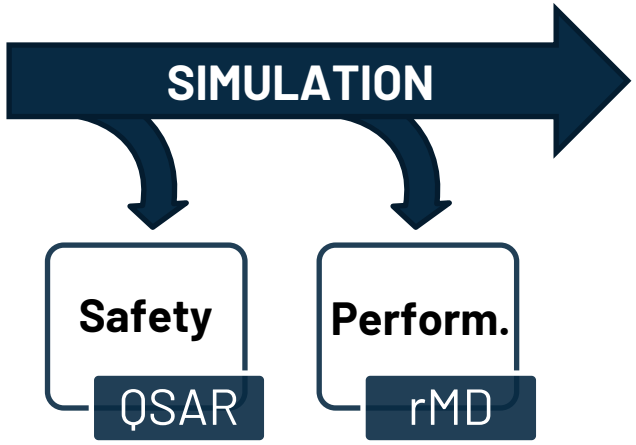
The Challenge:
Predict LCA for the entire life cycle

Platform – Input

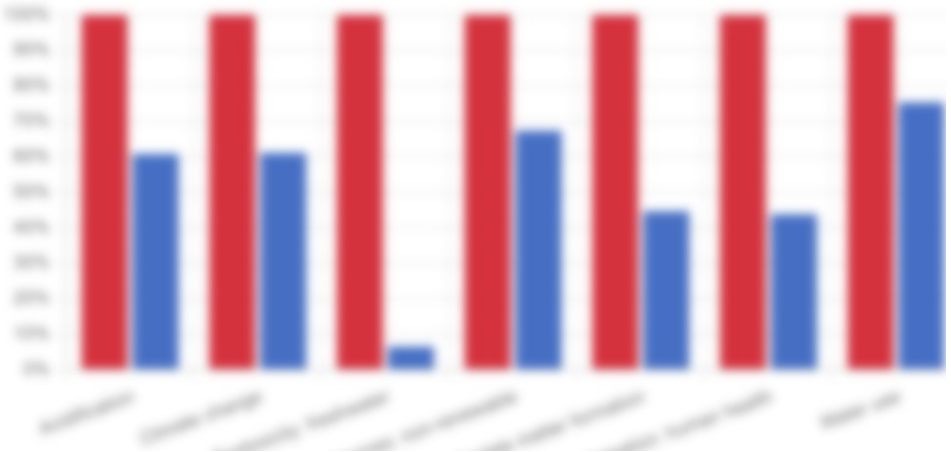


n1c2ccccc2[nH]n1

SMILES CODE
(or CAS)



Platform – Output



ENVIRONMENTAL IMPACTS
Cradle-to-Grave

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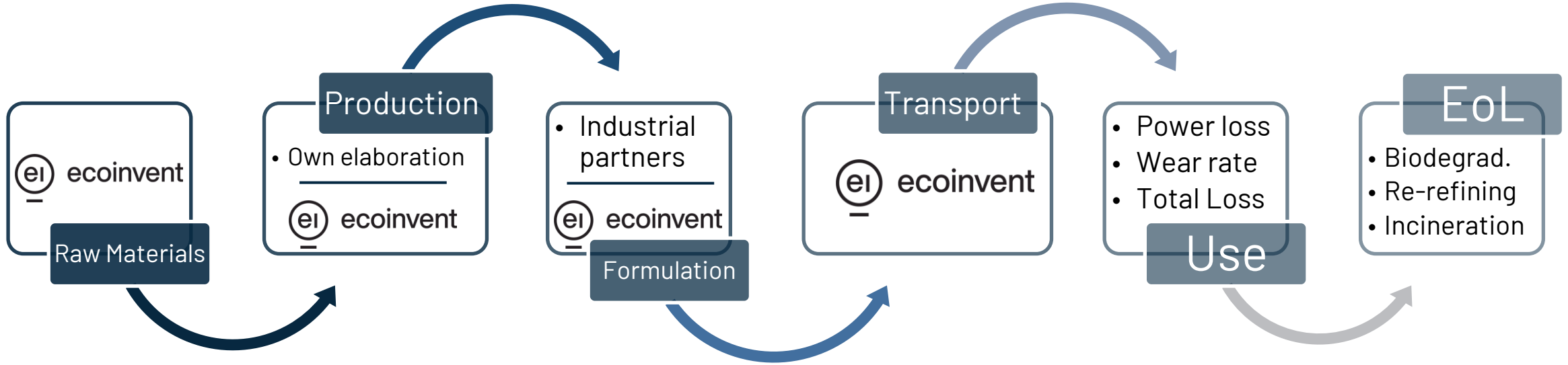
The Challenge:
Predict LCA for the entire life cycle of lubricants



Impacts (rule of thumb)

33%

66%

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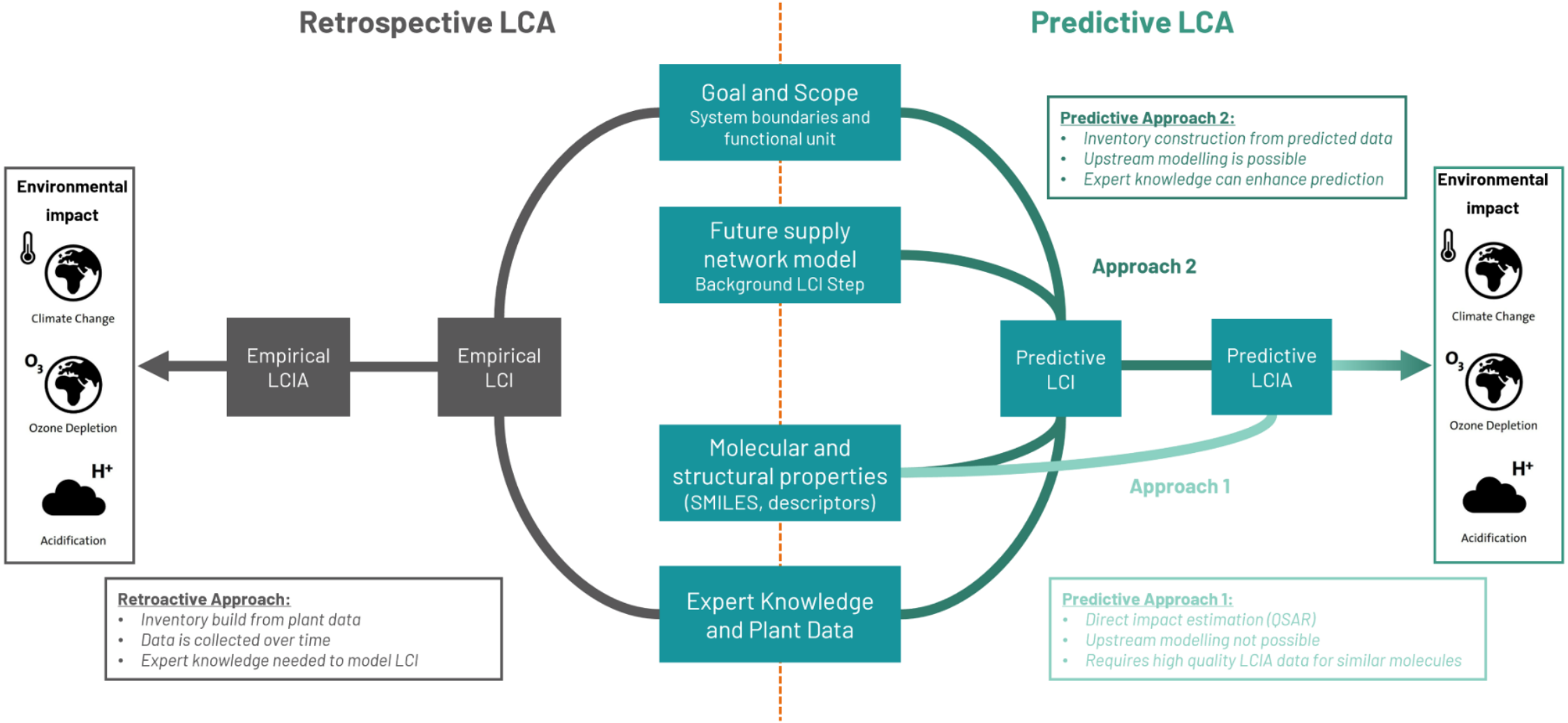
Raw Material Extraction and Production: The case of tolyltriazole (cradle-to-gate)



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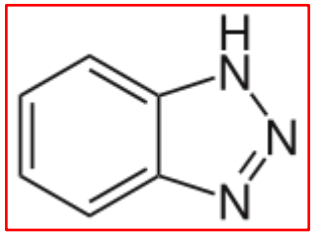
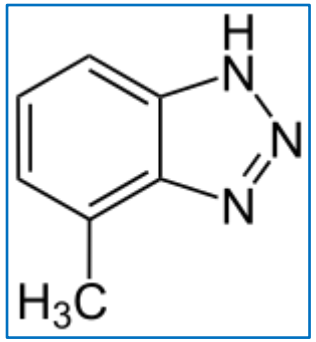
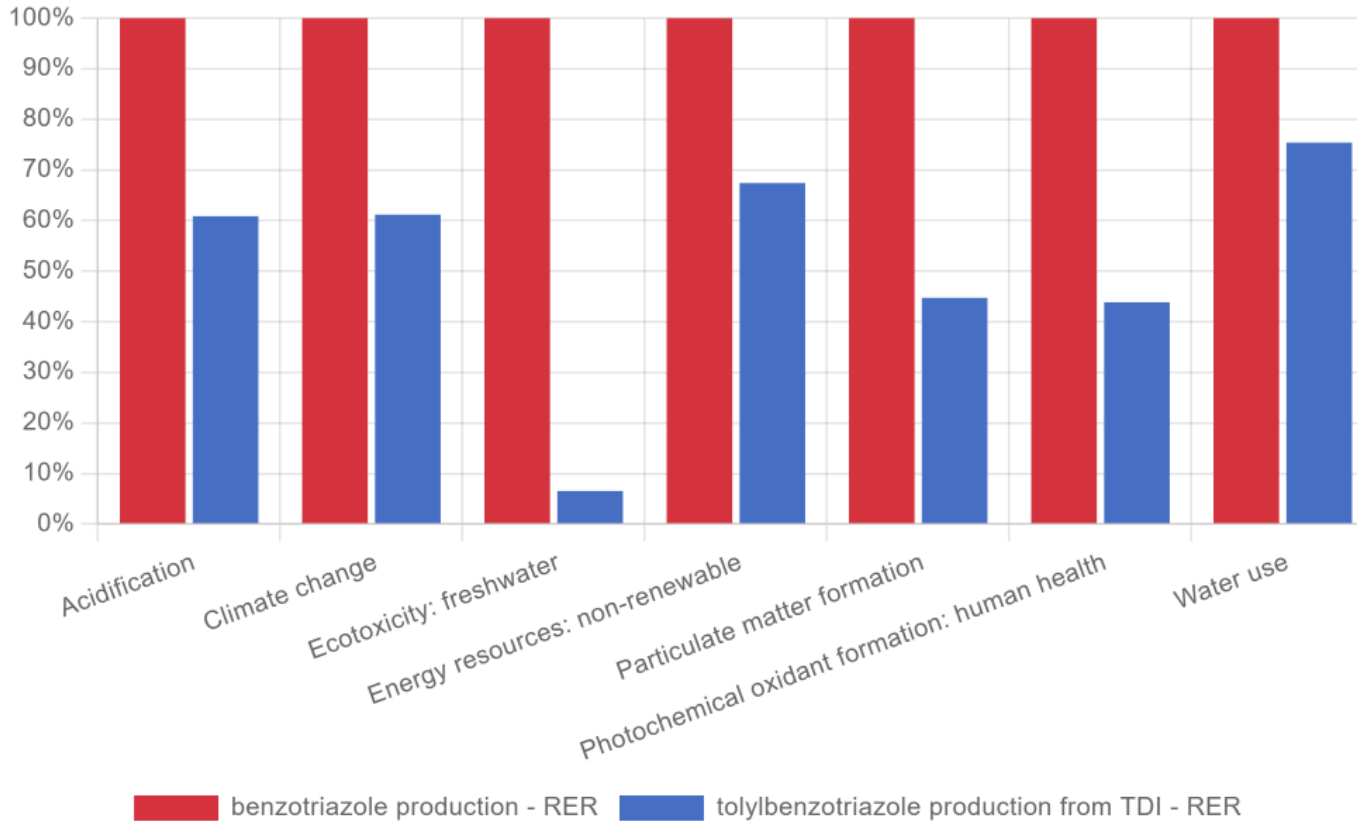


SSbD base case



SSbD alternative



cradle-to-gate, referenced to 1 mol of product, ecoinvent 3.11, EF 3.1 LCIA

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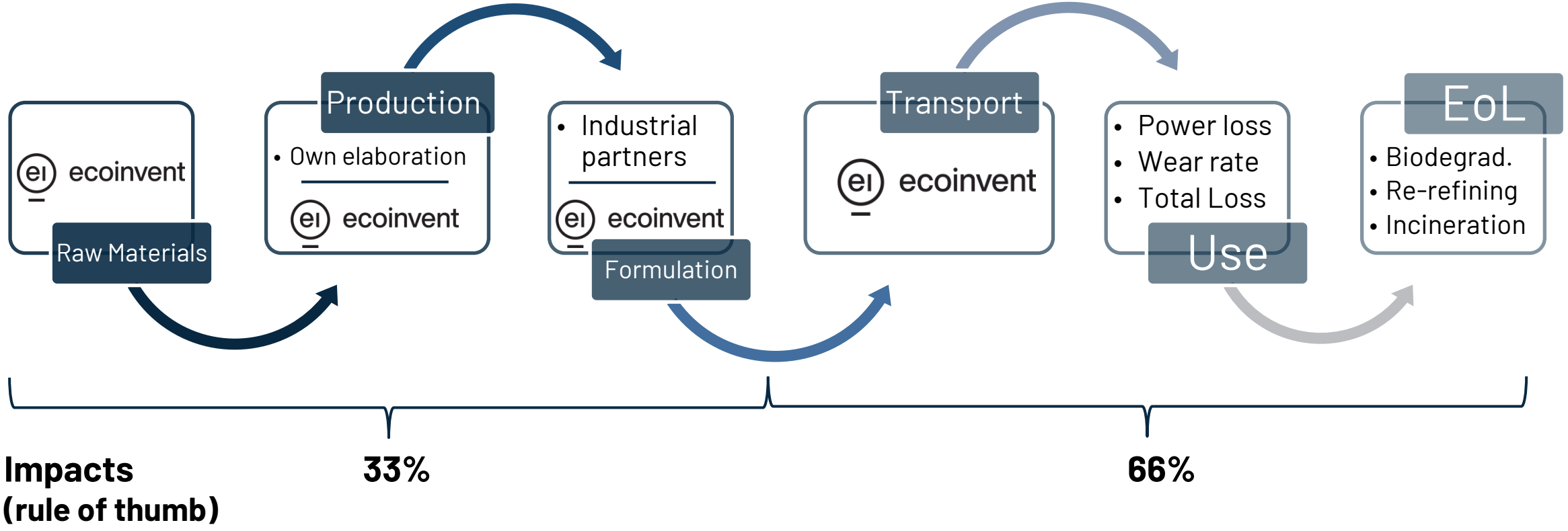

This is just production, see me at the poster for more!

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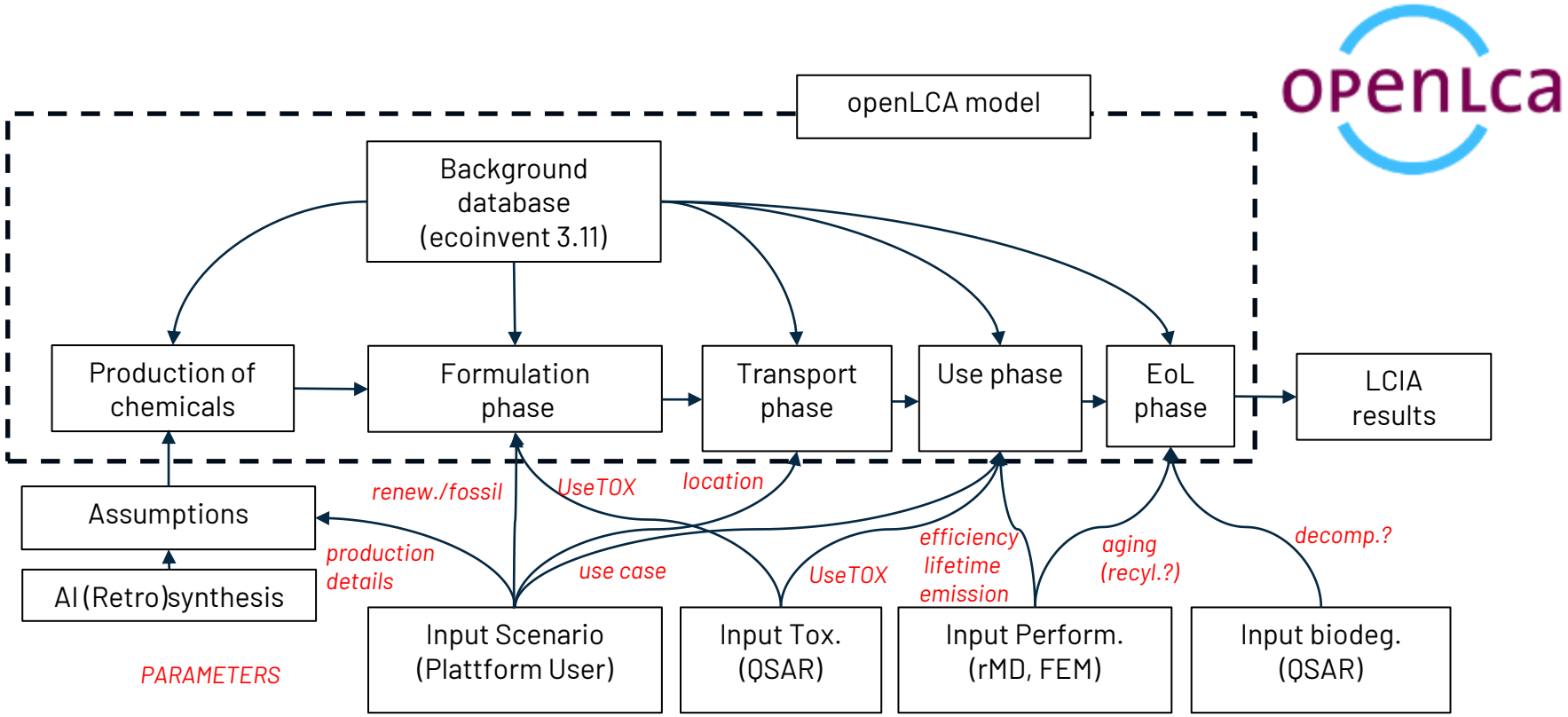
FÚLL LIFE CYCLE WITH PARAMETERS



Parametrized LCAs allows fully integrated SSbD approaches

→ openLCA's API will allow platform/AI interaction

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Thank you!

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