Safety and Sustainability – Assessments and Methodologies used in PERFECOAT

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High Performance Bio-based Functional Coatings for Wood and Decorative Applications

Safety and toxicity assessments and methodology

Painting a Bio-based Future with PERFECOAT – Achievements and current challenges of creating sustainable solutions in paints and coatings

27.08.2024, Andy Booth

Bio·based Industries Consortium

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Why conduct safety testing?

Safeguard human health
Reduce environmental impact
Regulatory compliance

Maintain optimal product performance

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Importance of early toxicity testing

- Facilitate early go-no go decisions:
  - Prevent time loss on developing (a group of) molecules with a non-favourable toxicity profile
  - Improved overall toxicity profile from starting materials - intermediates - final materials
- Give guidance for further testing
- Facilitate compliance with regulatory requirements
- Market introduction of safe bio-based products

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Task 6.1 - Chemical safety assessment

- Conduct a comparison of the chemical exposure risks between the new and existing materials.
- Identify and propose substitution of chemicals having the highest risk.

New generation and existing coating materials

Leaching Assessment (exposure)

OECD 442cSkin Sensitisation Assessment (hazard)

Risk assessment and ranking

Biopolymer coating development

Component selection

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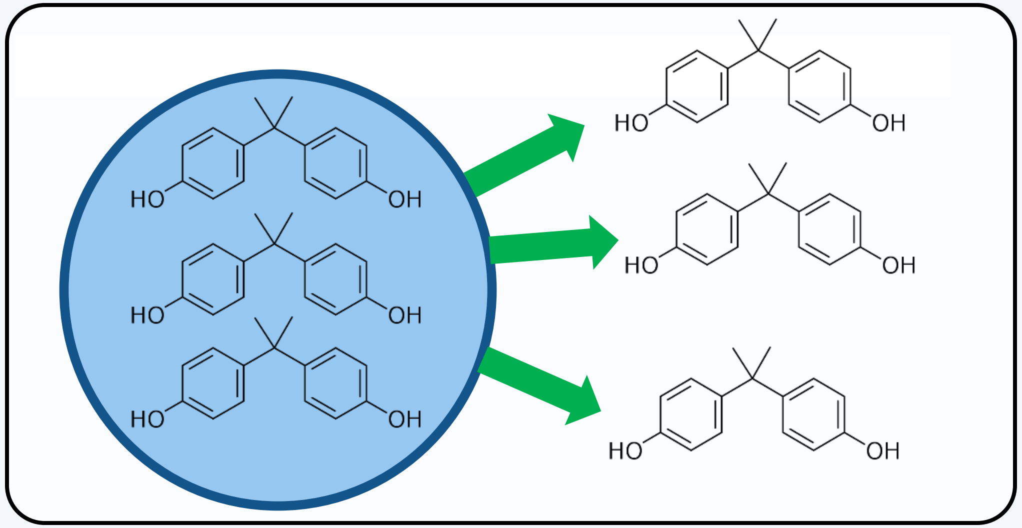
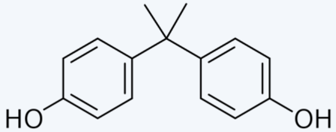
Leaching studies

Aqueous leaching

(Additives, residual chemicals, monomers)



Coating material on glass slide



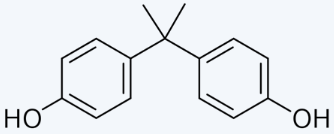
Bisphenol A

(example ingredient)

LC-MS Analysis

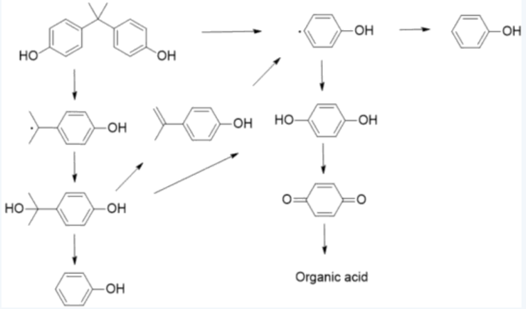
Target and non-target screening

Target



Bisphenol A

Non-target



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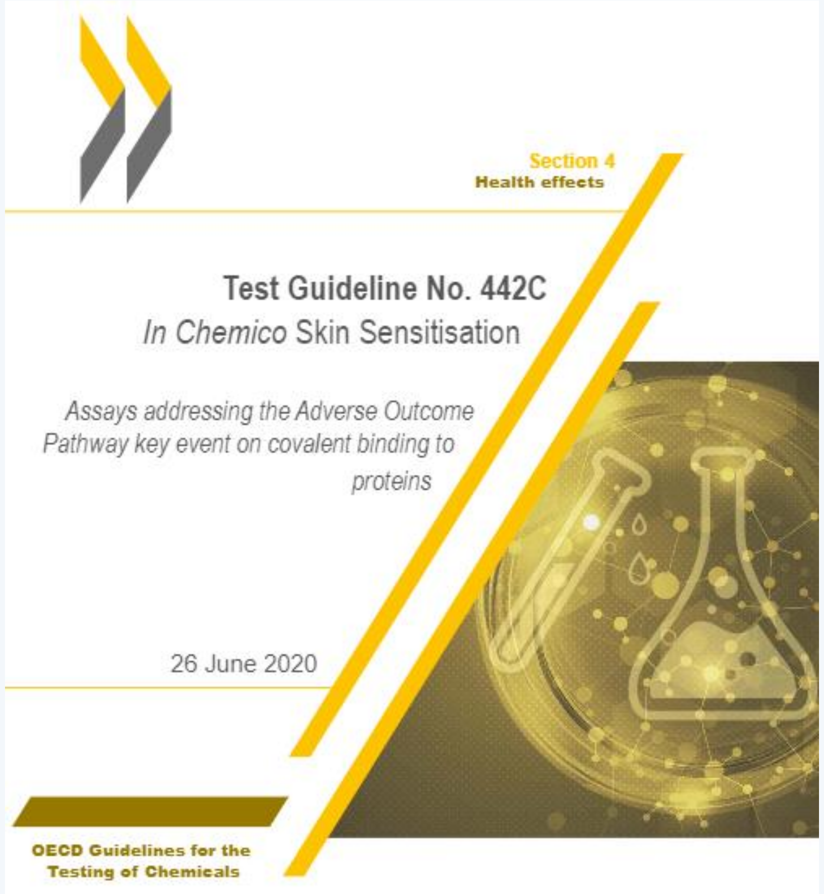
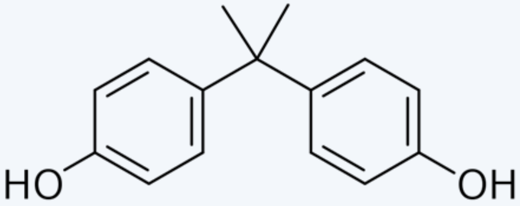
OECD 442c – Skin Sensitisation





Bisphenol A

(example ingredient)

An in *chemico* procedure (Direct Peptide Reactivity Assay – DPRA) used for supporting the discrimination between skin sensitisers and non-sensitisers.

Results for single chemicals

- Results of the DPRA testing are in line with the other classifications.
- For some chemicals this is the first sensitisation data.
- For particle ingredients skin sensitisation cannot be determined with this method

Summary from the skin sensitisation testing and comparison to existing classifications

Constituent Type	Name	CAS	Classification	CLP notifications (% of all)	Effects in-vivo (REACH)	DPRA - Skin Sensitisation (PERFECOAT)
Modifier	Calcium carbonate ($CaCO_3$)	471-34-1	Skin Irritant 2	Skin Irritant 2 (10%)	N	NA
Pigment	Titanium dioxide (TiO_2)	13463-67-7		Skin Irritant 2 (<0.1%)	N	NA
Defoamer	Polydimethylsiloxane	63148-62-9		Skin Irritant 2 (1.6%)	NA	NA
Coalescent	Propylene glycol propyl ether	1569-01-3	Skin Irritant 2	Skin Irritant 2 (20%)	N	Low
Photoinitiator	Irgacure 184	947-19-3		Skin Irritant 2 (0.1%)	N	Minimal
Diluent	TMPEOTA	28961-43-5		NA	Y	High
Main resin	Epoxyacrylate	55818-57-0	Skin Irritant 2 Skin Sensitizer 1	Skin Irritant 2 (6.5%) Skin Sensitizer 1 (92%)	Y	NA
Surfactant	Disponil SLS 101 Special	111072-31-2	Pre-registration			High
Surfactant	RHODAFAC RS/710-E	9046-30-5	Not in the database			Low
Surfactant	AEROSOL A-102E	68954-91-6	Skin irritant	Skin Irritant 2 (82%)	NA	High
Surfactant	Imbentin-T/120	9043-30-5	Skin irritant	Skin Irritant 2 (21%)	NA	Low
Surfactant	Emulsogen EPN 287	?	Not in the database			Minimal
Surfactant	Polirol AL 1347	?	Not in the database			Moderate

Safer by design

Example leaching ranking

No.	Compound/Component
1	Disponil SLS 101 Special
2	RHODAFAC RS/710-E
3	Emulsogen EPN 287
4	Polirol AL 1347
5	Imbentin-T/120
6	AEROSOL A-102 E
7	$CaCO_3$
8	TiO_2
9	Propylene glycol propyl ether
10	Irgacure 184
11	Trimethylolpropane ethoxylate triacrylate
12	Polydimethylsiloxane
13	Epoxyacrylate

Example toxicity ranking

No.	Compound/Component
1	Disponil SLS 101 Special
2	Epoxyacrylate
3	Emulsogen EPN 287
4	Trimethylolpropane ethoxylate triacrylate
5	Polydimethylsiloxane
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8	TiO_2
9	Propylene glycol propyl ether
10	Irgacure 184
11	AEROSOL A-102 E
12	Imbentin-T/120
13	RHODAFAC RS/710-E

High leaching + high toxicity

Med/low leaching + med/low toxicity

Low leaching + low toxicity

Example toxicity ranking

No.	Compound/Component
1	Disponil SLS 101 Special
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9	Propylene glycol propyl ether
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11	AEROSOL A-102 E
12	Imbentin-T/120
13	Irgacure 184

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Summary & Reflections

- There a many ways of conducting a safety assessment and these should be selected on a case by case basis
- Standard methods increase the comparability of different data sets and increase robustness
- The approaches outlined here are cost effective and high throughput methods – potential for widespread use
- The method uses only analytical chemistry, no animals, cells or biological material

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Environmental impact assessments in Perfecoat

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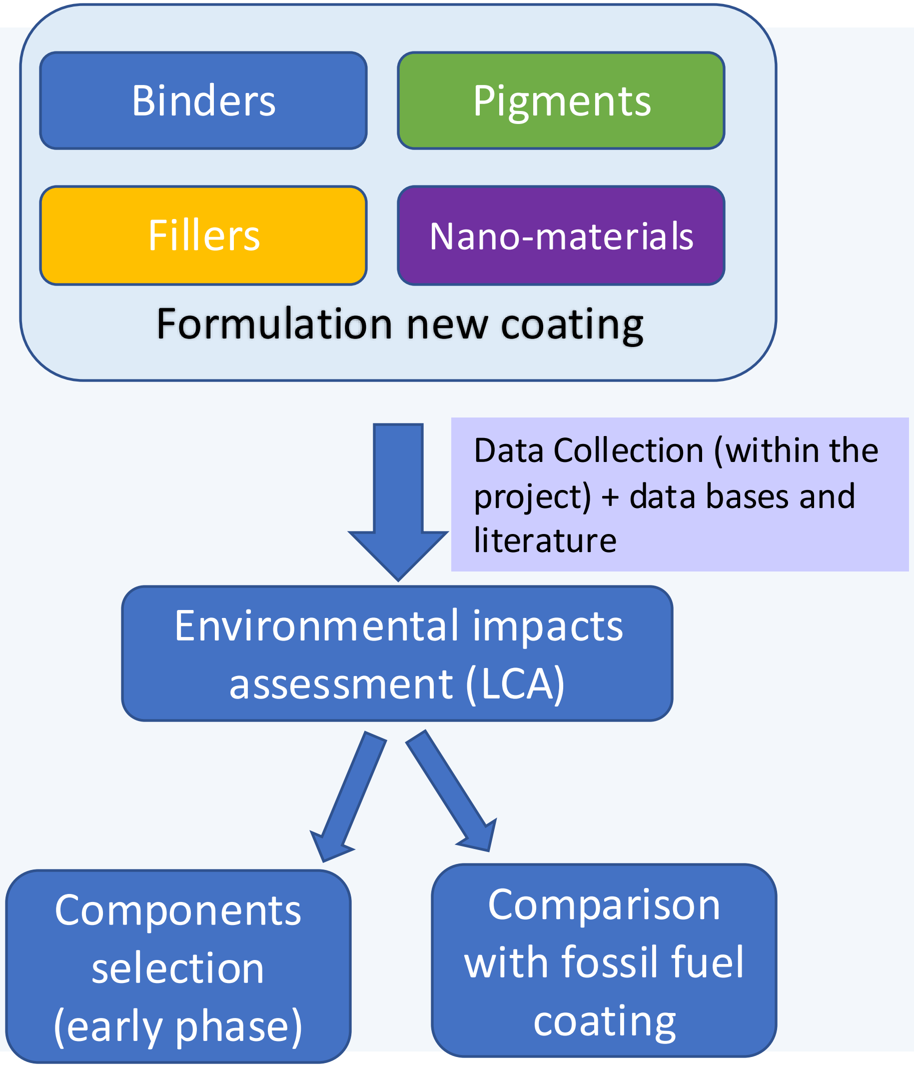
Environmental impact (LCA)

Objectives

- Life cycle assessment is used to assess the entire value chain (from feedstock to ingredients production and final coating formulations).
- Communicate results to work packages involved in the development to further optimise the proposed strategies with respect to environmental criteria.
- Select components entering the final formulation
- Compare new concepts with a standard fossil-based counterparts.



Scope definition

- Analyze environmental impacts of biobased ingredients and new coatings (UV curable and waterborne) and compare them with their fossil based counterparts.
- New coating formulations should have similar performance to the existing (fossil based) control paints.
- The functional unit of the study is set to 1 kg of product
- Only ingredients present in a quantity greater than or equal to 1% will be included according to UNEP/SETAC guidelines.

Life cycle inventory and impacts modellling

- Data was collected from industry partners, laboratory tests and relevant sources (e.g., Ecoinvent databases, literature, etc.).
- Models have been used to estimate inputs for upscaled production.
- Life cycle impact assessment step was conducted using the software SimaPro and the impact assessment methods such as EN 15804+A2, EF3.0, CML2.
- The greenhouse gases emissions have been the focus so far, but other impact categories have been analysed

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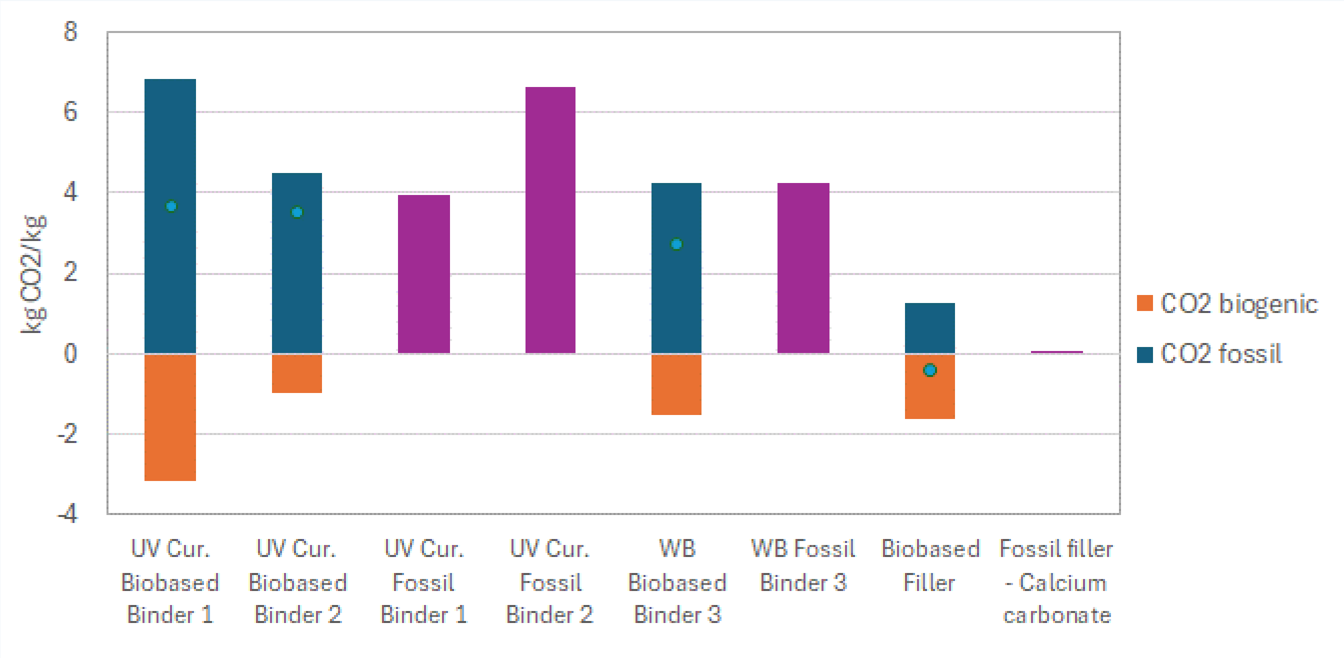
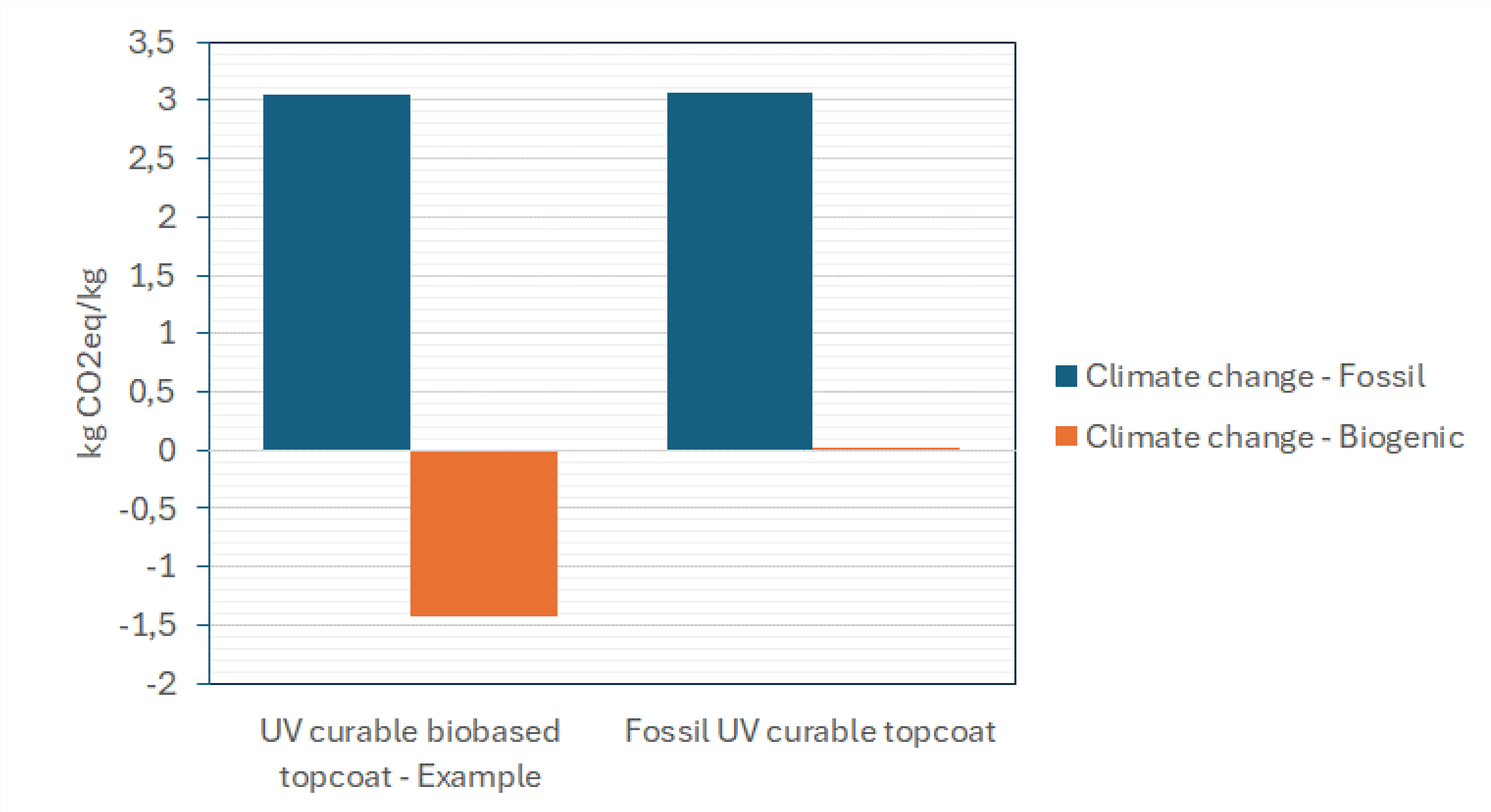
Few examples of LCA results on ingredients



- These results are based on estimates from models for industrial production, taking into account possible energy and solvent recovery.
- Chemicals and energy inputs (e.g., compressed air, steam, mixing, and homogenization) are significant hotspots.
- The results are only indicative at this stage as we are still at TRL 3-5.
- These results are encouraging and indicate that with further optimizations, the new biobased ingredients can outcompete certain fossil-based counterparts.

Comparison UV curable coatings
Example of topcoat formulation



Take home message

- Biobased ingredients and coatings have been developed using LCA to guide the development and minimise environmental impacts
- Although still at low TRL and without an extensive optimisation, biobased products are competitive in terms of carbon footprint compared to conventional fossil counterparts
- What can LCA do?
  - Understanding your products' environmental impacts and identify hot spots
  - Product improvement at the design stage
  - Comparison of products and production routes
- Keep in mind the uncertainty in the data used especially at low TRL

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Social acceptance and social study of biobased solutions in Perfecoat

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Objectives

Identify and assess the potential social impacts of the new solutions, with a special focus on social acceptance and perceived transition potential.

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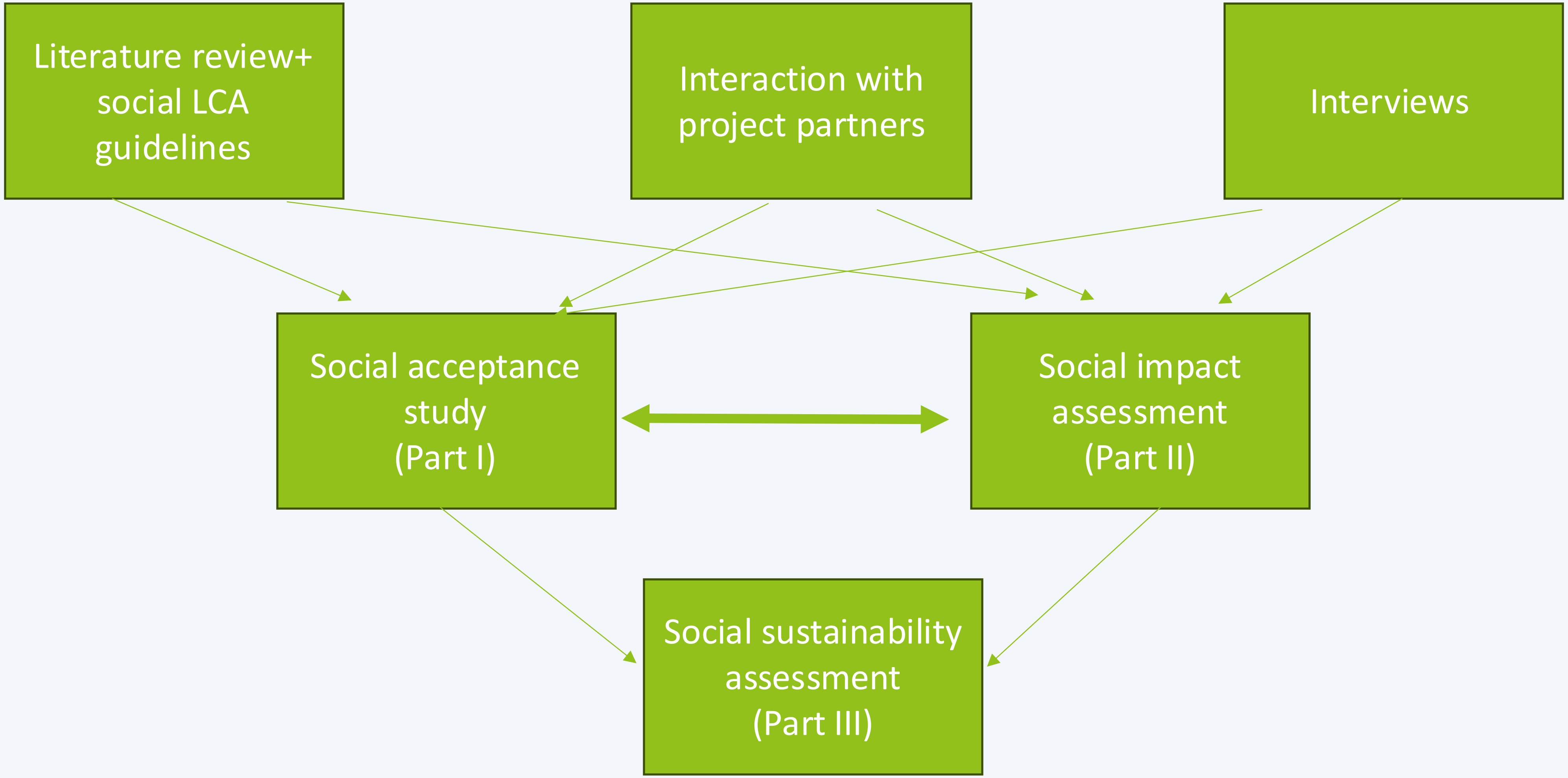
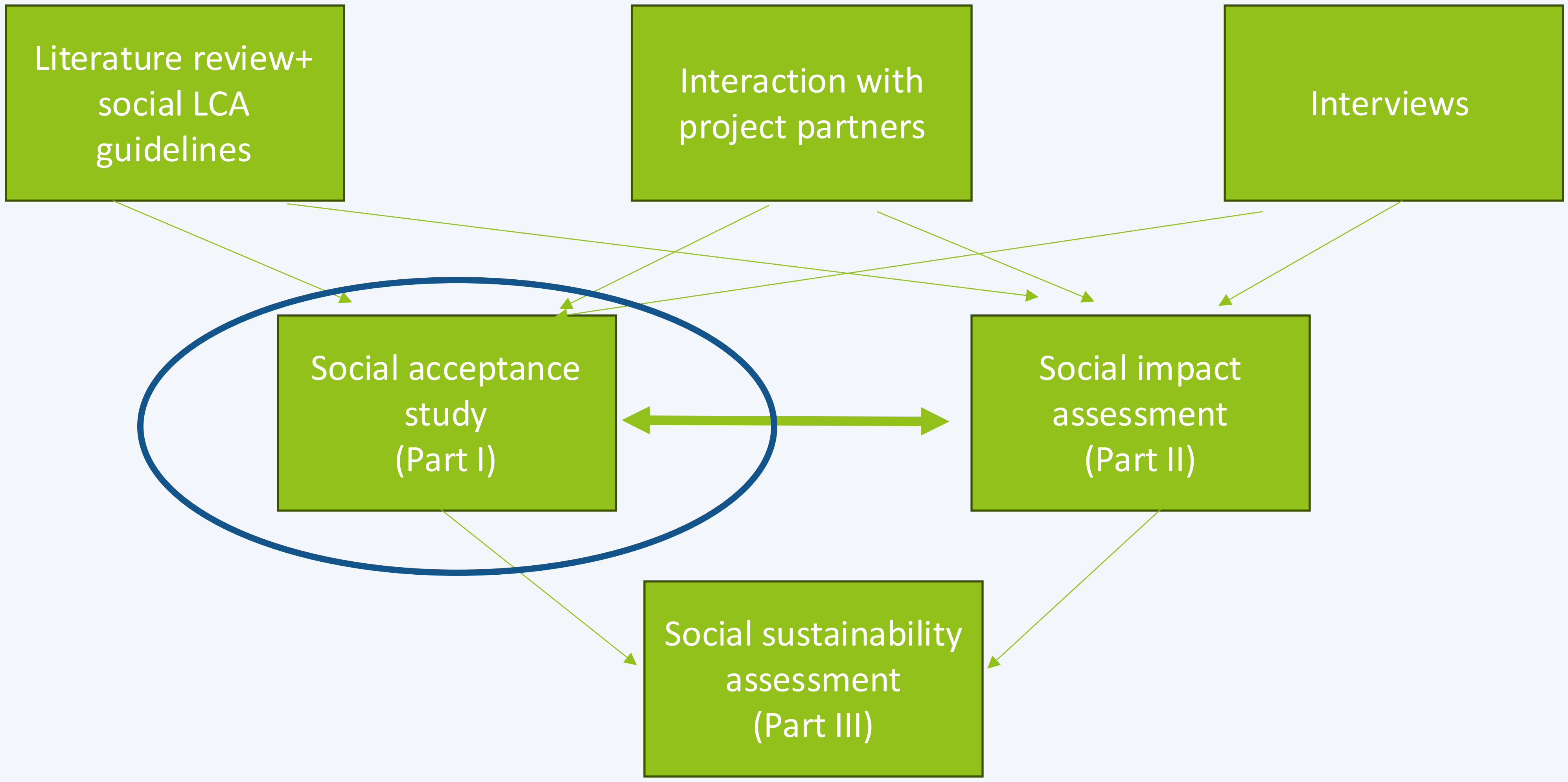
Social sustainability: methodology



Social sustainability: methodology



Social acceptance

- **Socio-political acceptance**:
  - Drivers at an overarching policy level (e.g., EU Green Deal, bioeconomy strategy and circular economy action plan of the EU, etc.) are present
  - Perceived lack of direct incentives, sustainable innovations is up to the industry actors.
  - Mixed effects of eco-labels

Images from PowerPoint archive

Social acceptance

- **Market acceptance**:
  - Increased importance to document sustainability
  - Lack of explicit and specific sustainability targets, to guide suppliers – with some exceptions
  - High costs and prices constitute a major barrier
  - Users still need to be convinced on several coating functionalities.
  - For the value chain actors, compatibility of new, bio-based solutions with the existing plant and production processes is crucial → If any radical process changes are required these will be both costly and time-consuming.


Image from PowerPoint archive

Social acceptance

- **Community acceptance**:
  - Land use and the risk of indirect land use change matters
  - Reliable supply of sustainably produced biomass is necessary,
  - Transparency regarding raw material origin is required
  - Human rights and labour rights are assumed to be in compliance

Image from PowerPoint archive

Final reflections

- Few studies on social sustainability of the biobased coatings
- Challenging data access
- Complex value chains
- Early-stage development
- Increasing focus on social sustainability and sustainability in general
- Close follow-up and interaction are crucial

Thanks for your attention!

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