Quantitative-based and case-specific MCDA methodology for SSbD multioptimal solutions including stakeholders' perspective

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SSbD implies a Multidimensional, quantitative and case-specific methodology

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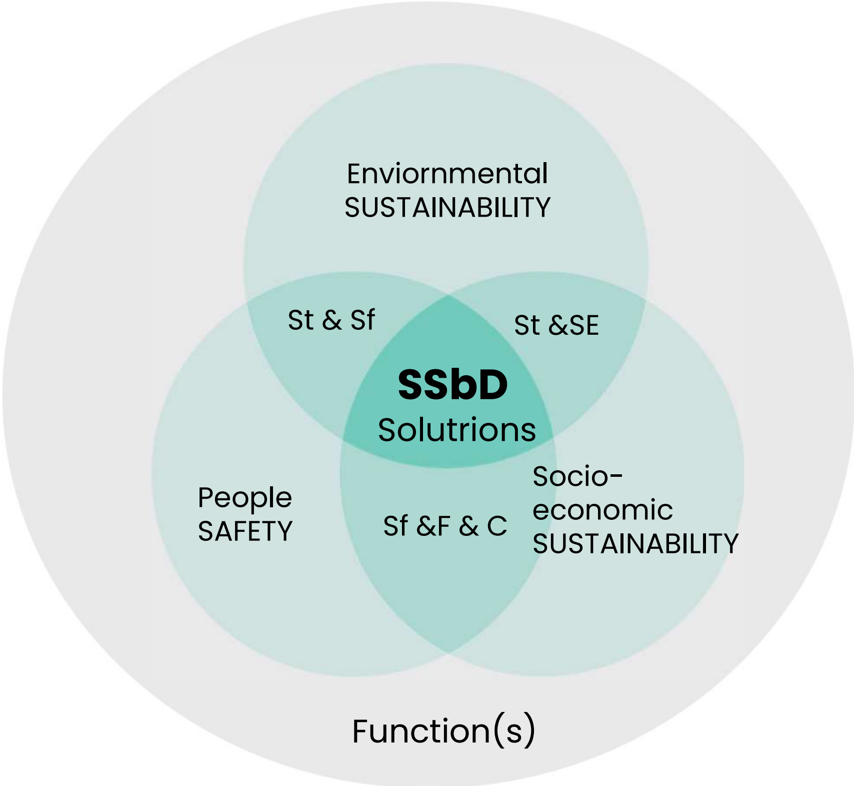
SSbD: MULTIDIMENSIONAL AND HOLISTIC



SSbD implies a multidimensional approach

Safe and Sustainable by Design (**SSbD**) **solutions** need to comply with the requirements in all dimension:

- Health
- Environment
- Economy
- Society
- (Function)

This implies a **holistic approach** in the safety and sustainability assessment challenge

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A QUANTITATIVE APPROACH TO SSBD: WHY?

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A QUANTITATIVE APPROACH TO SSBD: WHY?

- to reduce the level of arbitrariness in decision making
- to refer to robust and aknowledged reference levels
- to allow ordering and ranking
- …

A QUANTITATIVE APPROACH TO SSBD: IS IT POSSIBLE?

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A QUANTITATIVE APPROACH TO SSBD: IS IT POSSIBLE?

Safety, environmental- and socioeconomic-sustainability, functionality... can be measured?

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CASE-SPECIFIC MEASUREMENTS AND ASSESSMENTS: WHY?

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CASE-SPECIFIC MEASUREMENTS AND ASSESSMENTS: WHY?

Because it allows for clearer and better comparisons made on the same comparative basis

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HURDLES IN R&D CHALLENGING SSBD

- Unavailability of case specific data
- Limited amount of data that can be generated due to:
  - Resource limitations
  - Time constraints
  - costs

To make SSbD applicable to R&D in the framework of responsible innovation exploitation of resources, time and cost should be reduced to the minimum and sufficient

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Features Advantages and Requirements of the SSbD MCDA methodology

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FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

Feature / advantage ➡

QUANTITATIVE BASED

Allows for:

- objective assessments
- Comparison of design options performances within the same design case study
- Comparison of design options performances with benchmarks or other competing SSbD solutions

Feature / advantage ➡

CASE SPECIFIC

Generating data are contextualised and are representative of defined and controlled conditions, assumptions, cut-offs

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FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

Feature / advantage ➡

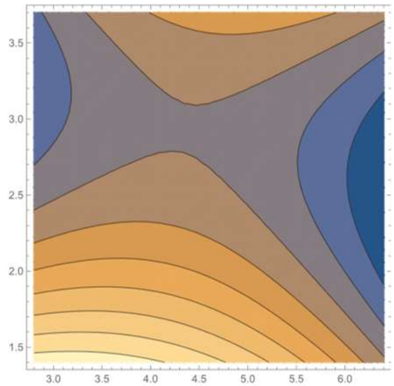
IS SUPPORTED BY DECISION SUPPORT IT TOOL (DST) POWERED BY SYMBOLIC AI ALGORITHMS

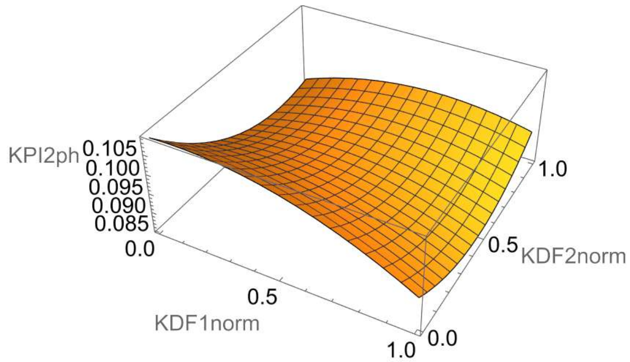
The analytical complexity is incorporated into the computational algorithm simplifying the decision-making process

Feature / advantage ➡

CAPTURES NON LINEARITIES

The MCDA DST captures KPIs non-linearities and KDFs interactions





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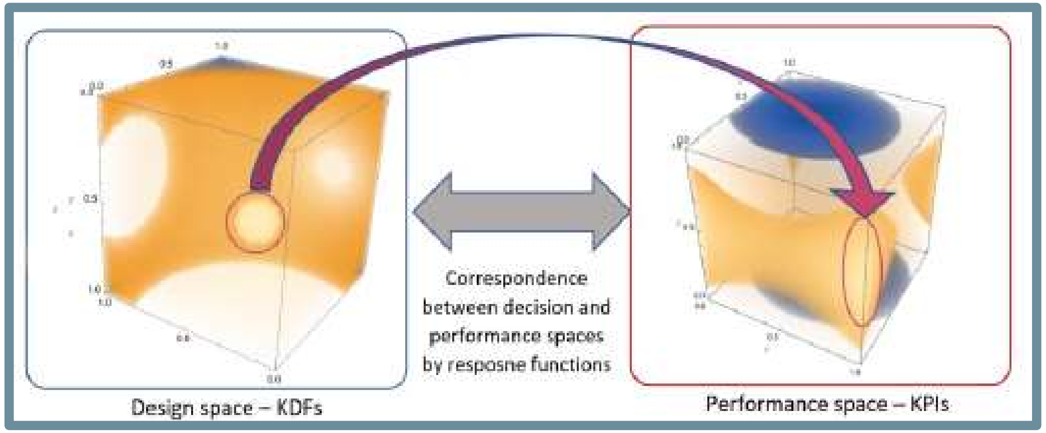
FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

Feature / advantage ➡

RELATES MULTIPERFORMANCE PROFILE TO DESIGN OPTIONS

From selected multiperformance level the corresponding design option(s) is provided



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FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

Feature / advantage ➡

ASSOCIATES MULTIPERFORMANCE TO P-CHEM FEATURES (PCF)

The association of an obtainable performance level to the PCFs:

- Enables more targeted and quantitative based grouping
- Enables Read-across
- Provides indications for future resarh optimisation and finding of alternatives
- Provides indications on modelling and development of mechanicistic interpretations (theories and modelling)

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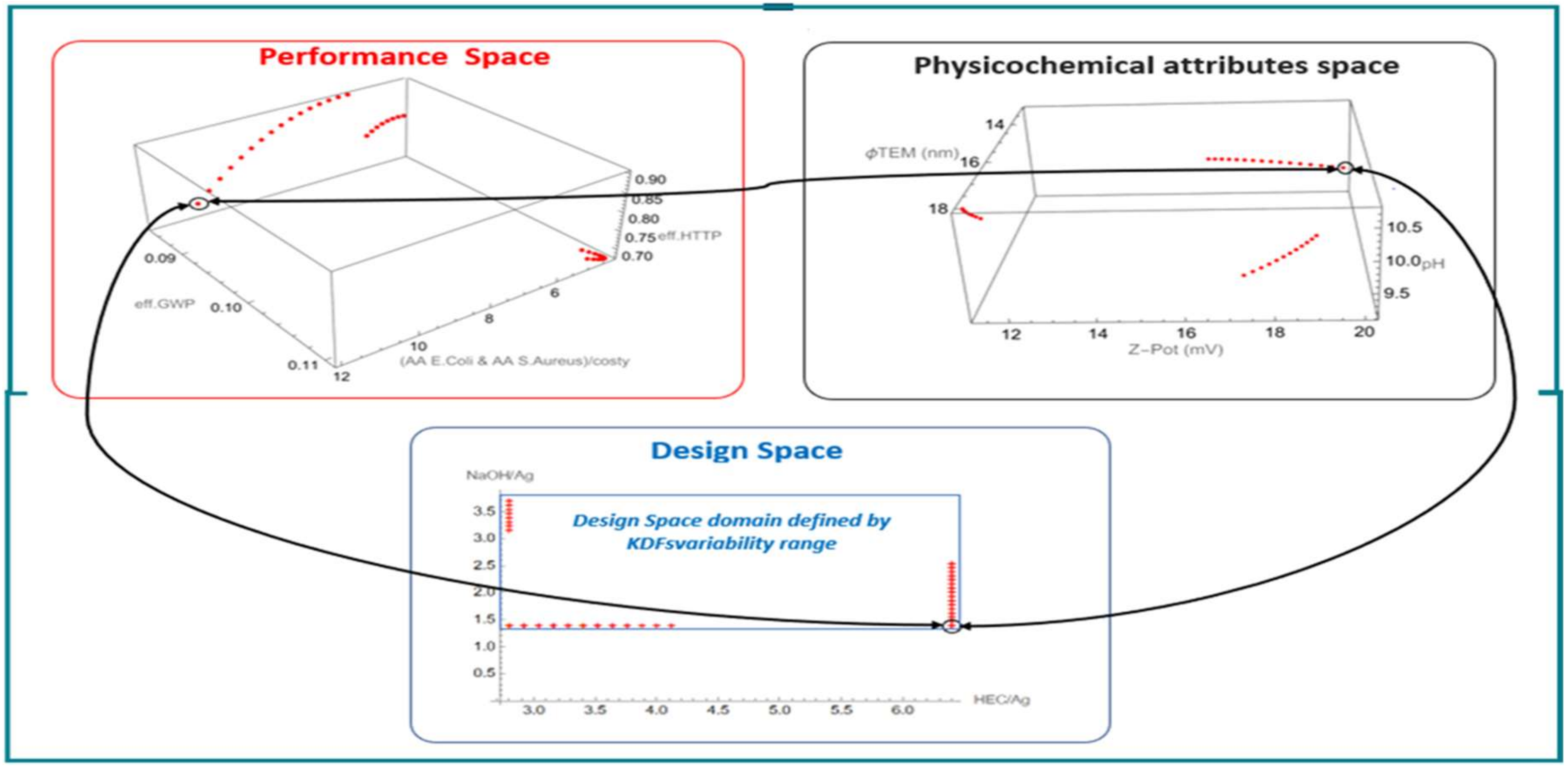
FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

ASSOCIATES MULTIPERFORMANCE TO P-CHEM FEATURES (PCF)



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FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

Feature / advantage ➡

HOLISTIC AND MULTIDIMENSIONAL

All dimensions: safety, environmental, economic, social and functional are considered simultaneously: it avoids discarding suitable design options by premature discarding due to sequential selection in different dimensions

Feature / advantage ➡

INCORPORATES STAKEHOLDERS (ACTORS) PERSPECTIVES

The set of suggested SSbD design options incorporates the stakeholders' profiles

Feature / advantage ➡

HUMANCENTRIC DECISION MAKING

Based on the suggested SSbD set of design options negotiation among different stakeholders is made possible based on quantitative evidence for taking informed decisions

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FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

Advantage ➡ **TACKLES COMPLEXITY THROUGH MODULARITY**

MCDA may be applied at different levels and sequentially: the complexity of each design case encompassing the whole NM Life Cycle may be approached by

- focusing on the KPIs multiplicity of each dimension
- treating each LC phase, separately and sequentially by applying the stage gate process

Requirement ➡ **REQUIRES A COMPLETE AND HARMONISED DATASET**

For each design case the set of safety, environmental, economic, social and functional KPIs measurements must be obtained in each dimension

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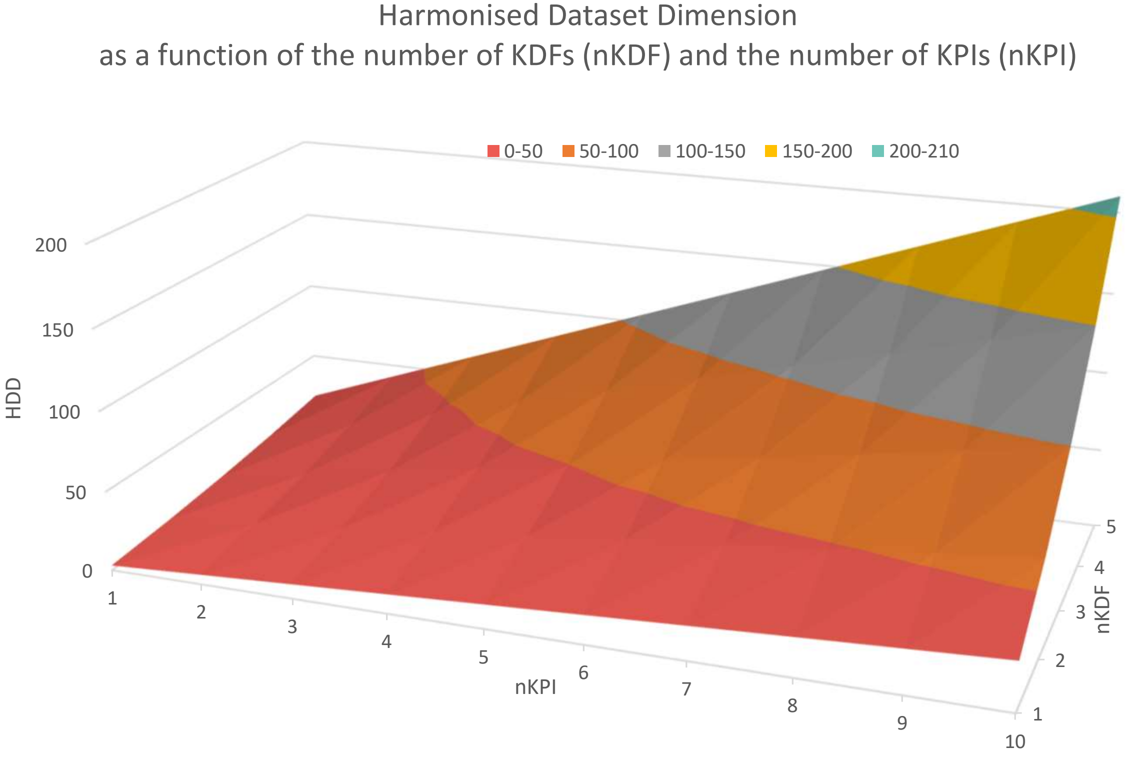
FEATURES, ADVANTAGES AND REQUIREMENTS OF THE SSbD MCDA METHODOLOGY

Requirement & Advantage ➡ MINIMISES THE BURDEN OF DATA GENERATION



A Minimum and sufficient amount of data are enough to run the MCDA For continuous Key Decision Factors (KDFs), The number of design cases (NDC) scales with the squared number of KDFs (nKDF), and the total harmonised dataset dimension (HDD) scales with the number of design cases times the number of KPIs (nKPI):

HDD=NDC x nKPI

HDD={[(nKDF)^2+3 x nKDF+2]/2} x KPI

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QUANTITATIVE APPROACH TO SSbD

TO MEASURE ⇔ TO QUANTIFY ⇔ TO COMPARE

Metrology requirements for quantification

1	2	3	4
Defined quantity	Unit of measurement	Measuring tool	Procedure (measurement method)
Define KPIs in all dimensions	Making use of standardized metrics / scoring	Making use of calibrated instruments and or validated models	Follow a standardized procedure and or modelling methodology

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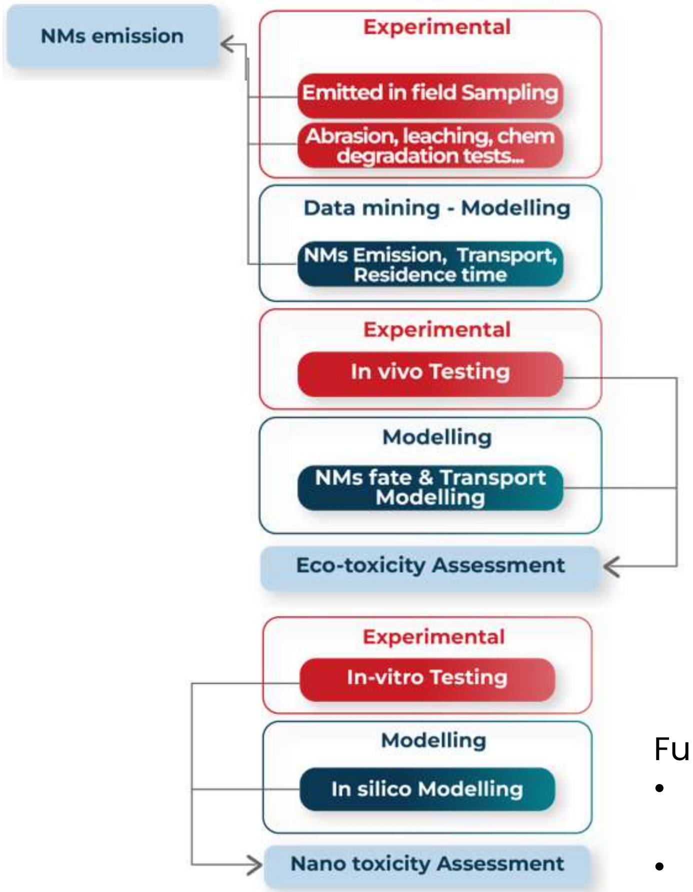
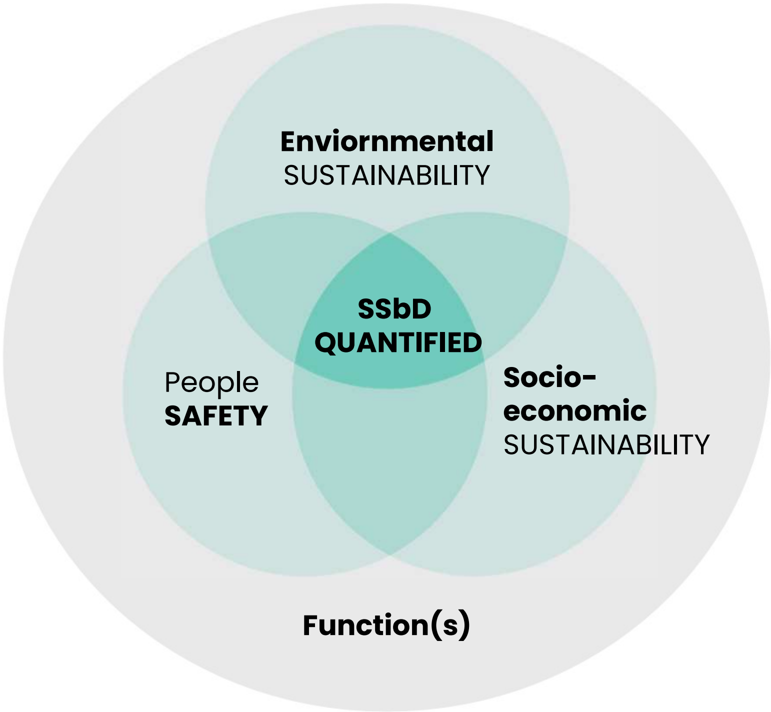
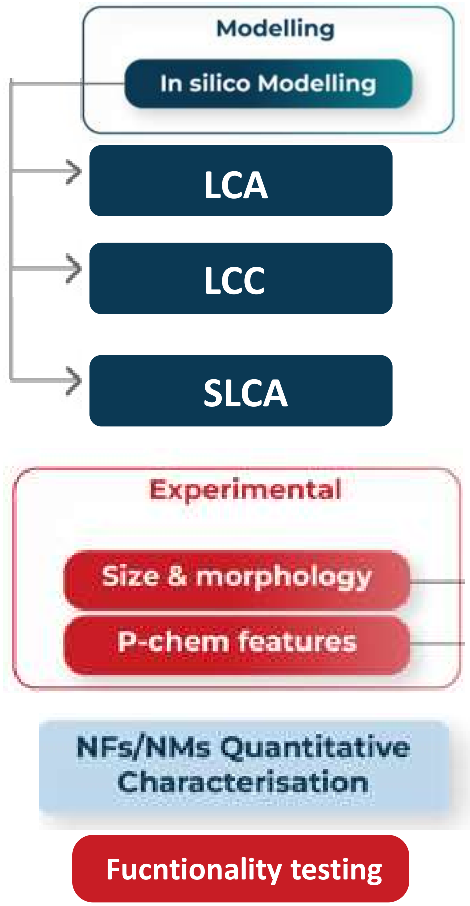
HOW TO MEASURE SAFETY, SUSTAINABILITY, FUNCTIONALITY?







Functions quantified by experimental testing, e.g

- Depollution by photo/thermocatalitic : quantify desctruction of pollutants(e.g. CECs) in specific conditions
- Antibacterial/antiviral: colony rediction count

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STANDARDS: METHODS, UNITS?

Environmental impacts:

- Life Cycle Assessment – **LCA**, ISO 14040-44
- Carbon footprint – **CFP**, ISO 14067

Economic:

- Life Cycle Costing - **LCC**

Social:

- Social Life Cycle Assessment – **S-LCA,** ISO 14075:2024

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MCDA within DMADV

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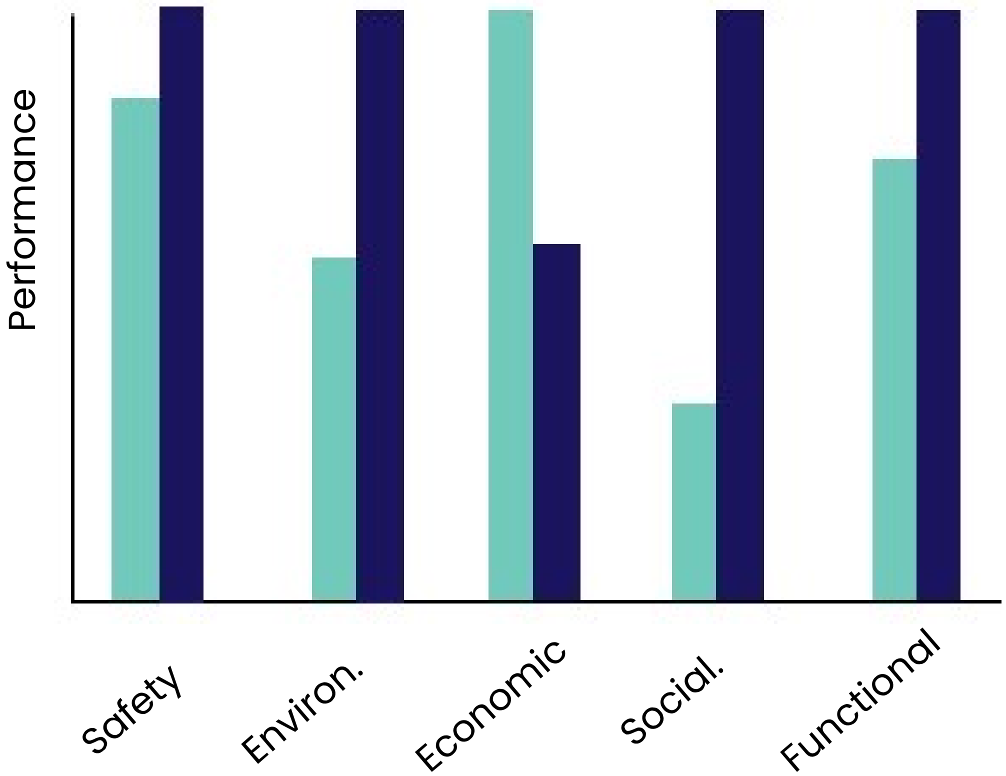
DECISION MAKING CONSIDERING MULTPLE DIMENSIONS TO COMPARE DESIGN OPTIONS

Design option A



Design option B

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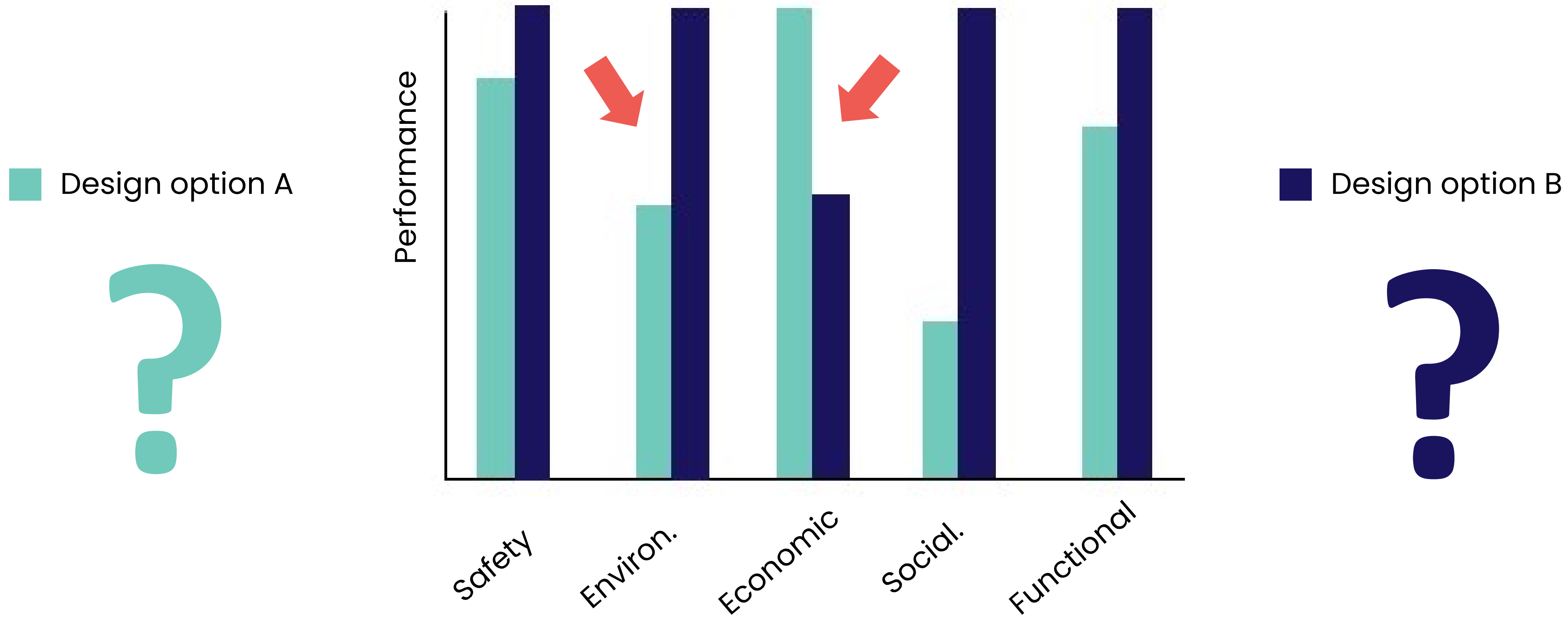
DECISION MAKING CONSIDERING MULTPLE DIMENSIONS: IS NOT TRIVIAL



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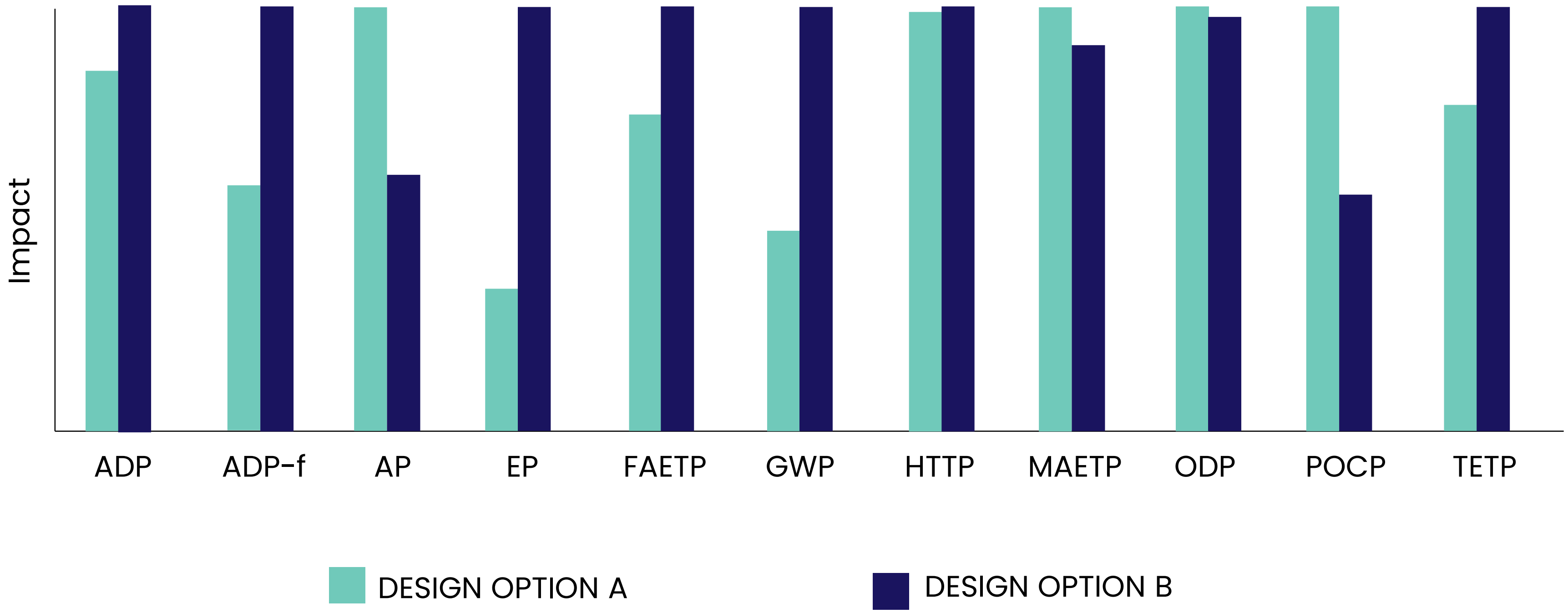
EVEN WHEN REFERRING TO A SINGLE DIMENSION DECISION MAKING IS NOT TRIVIAL: ENVIRONMENTAL KPIs



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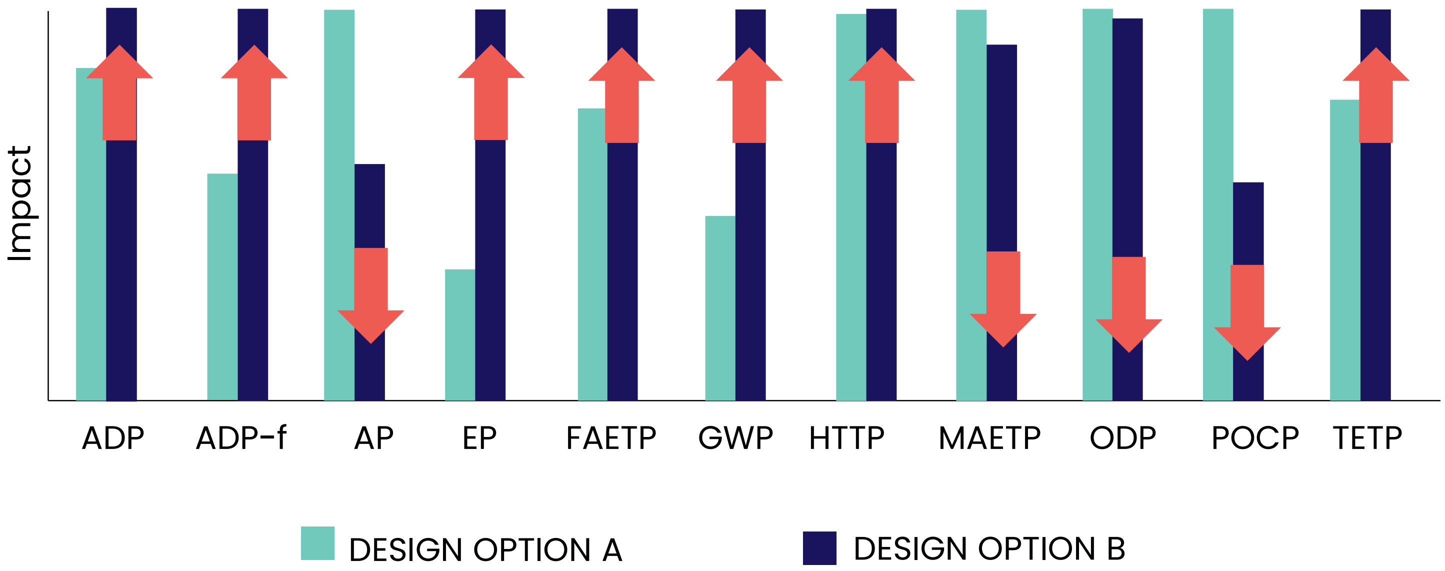
DIFFERENT DESIGN OPTIONS PERFORMANCES

How to deal with performance trends inconsistencies?
How to decide for the best design option?
May we compare different KPIs?
Have they the same importance?



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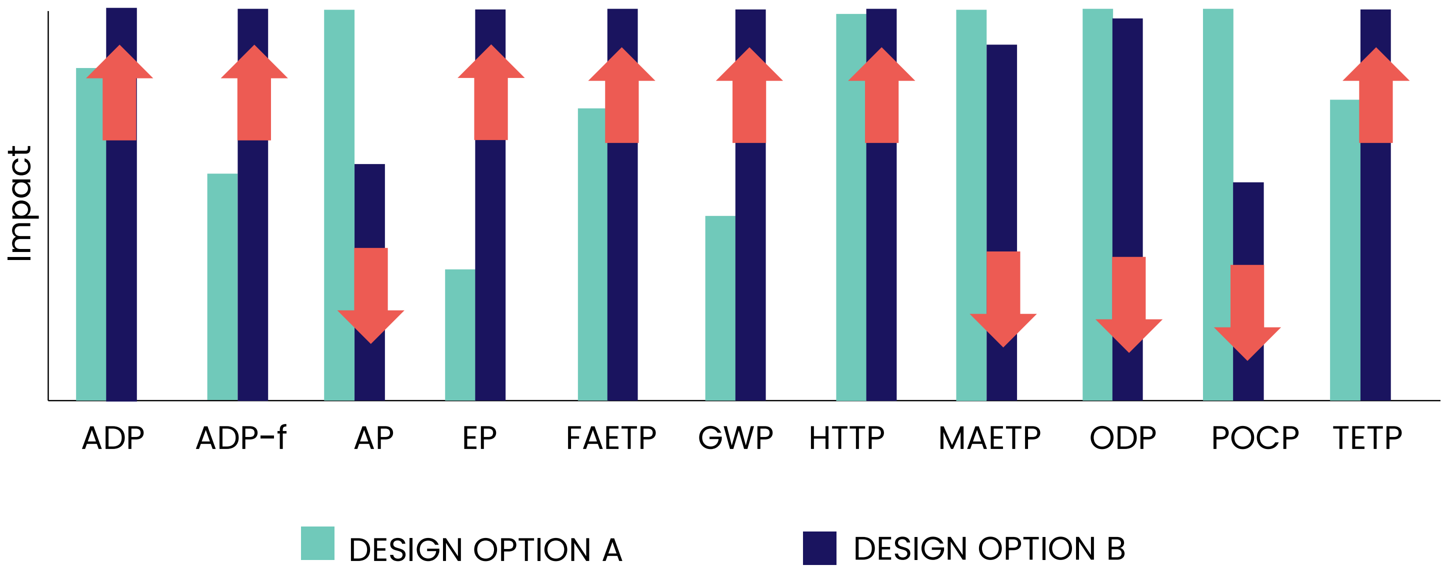
DIFFERENT DESIGN OPTIONS PERFORMANCES

How to deal with performance trends inconsistencies?
How to decide for the best design option?
May we compare different KPIs?
Have they the same importance?

Need of **MCDA**
Multi-Criteria Decision Analysis



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METHODOLOGY AND WORKFLOW FOR QUANTITATIVE AND CASE-SPECIFIC MCDA ENABLING SAFE AND SUSTAINABLE BY DESIGN (SSBD) SOLUTIONS

- Based on industrial **Six Sigma framework**
- Inspired by **standardised assessment methodologies**
- **Compliant** with the **framework for Safe and Sustainable by Design** chemicals and materials

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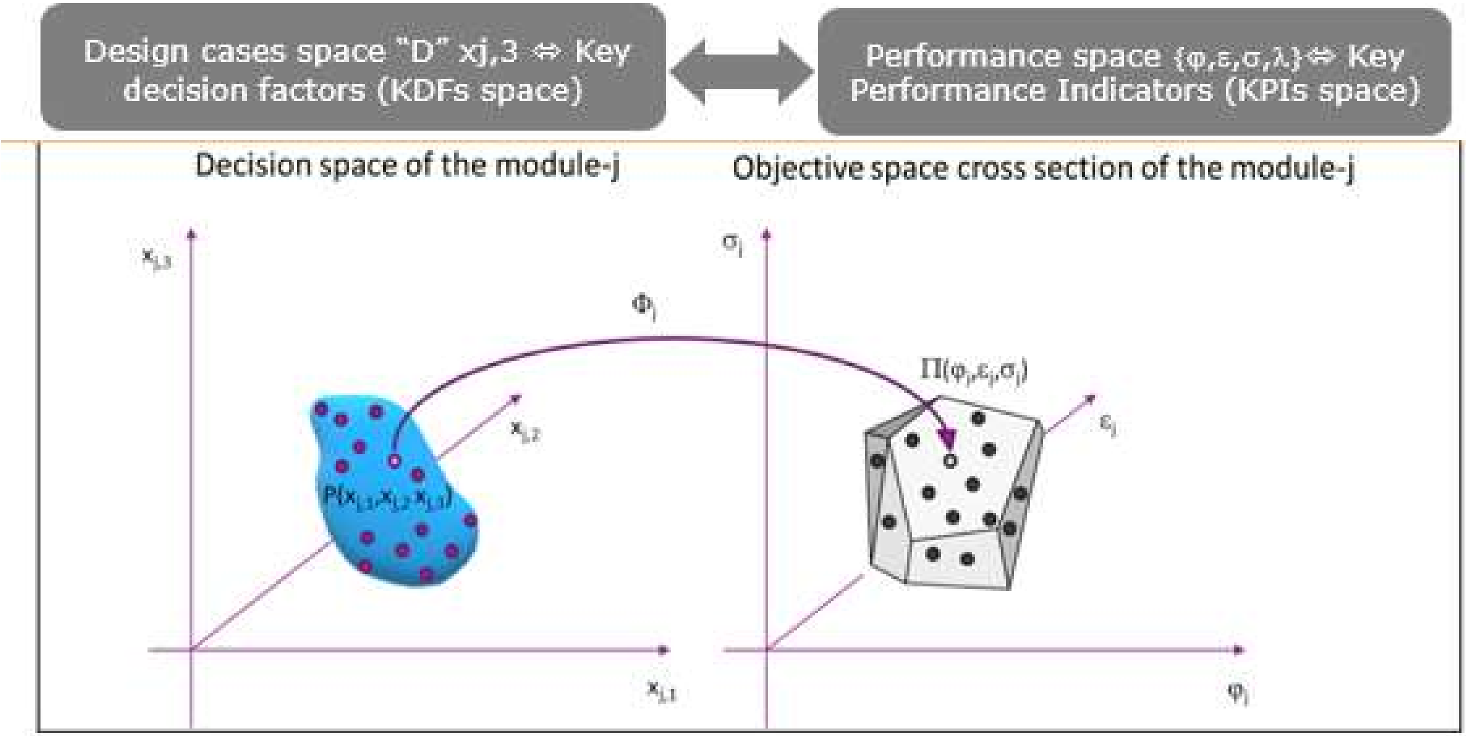
EACH DESIGN OPTION AFFECTS THE KPIS IN DIFFERENT DIMENSIONS



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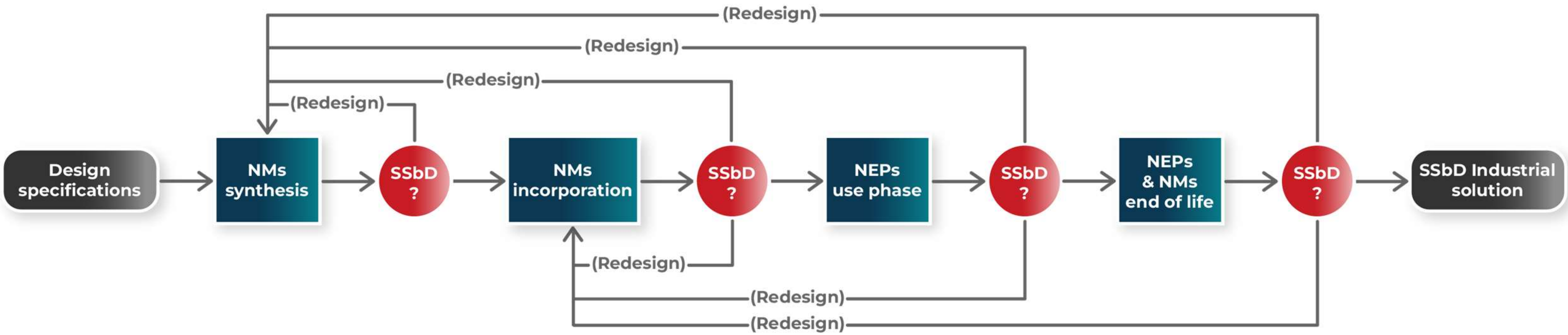
FROM DESIGN SPECIFICATIONS TO SSBD SOLUTIONS



Stage-gate process enabling rationalized design & redesign process

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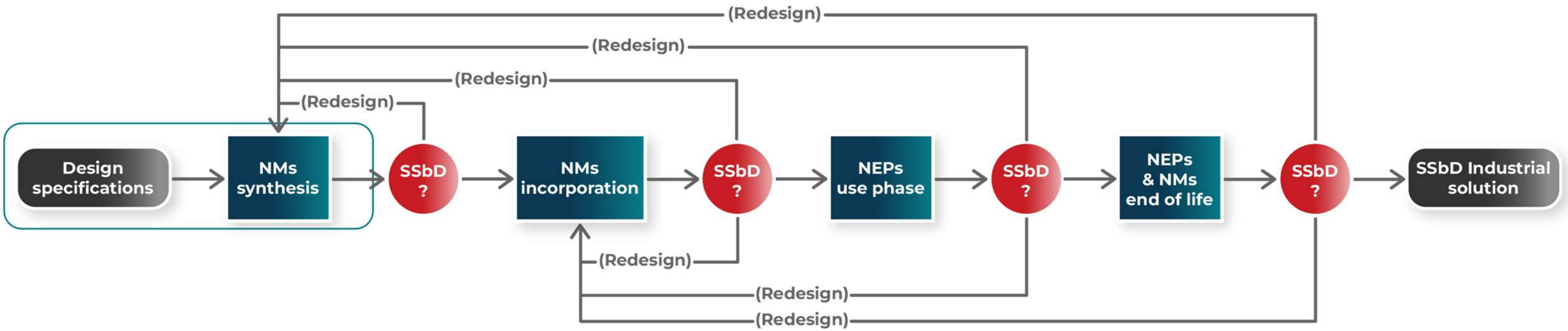
STAGE-GATE PROCESS FOR DESIGN & REDESIGN



Each LC may be treated separately through a **specific (sub-) case study**

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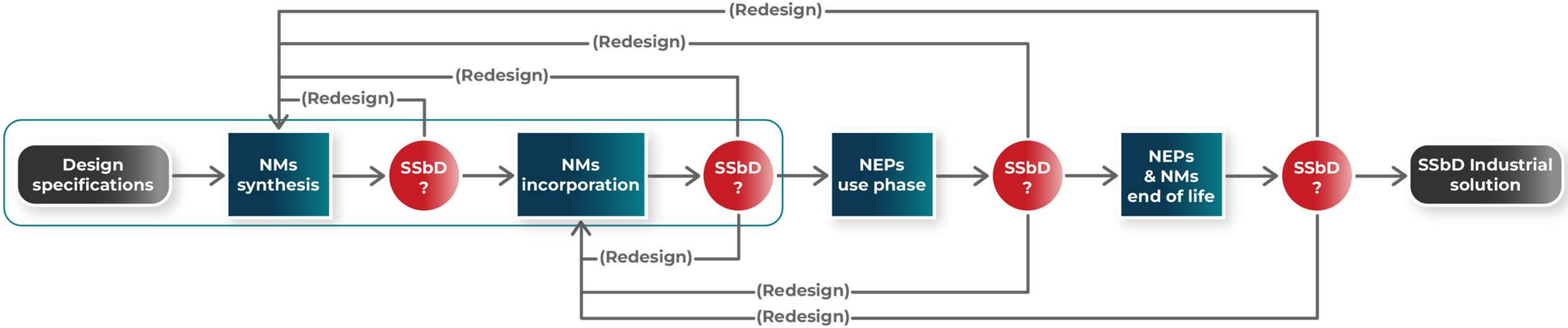
STAGE-GATE PROCESS FOR DESIGN & REDESIGN



Each LC may be treated separately through a **sequence of (sub-) case studies**

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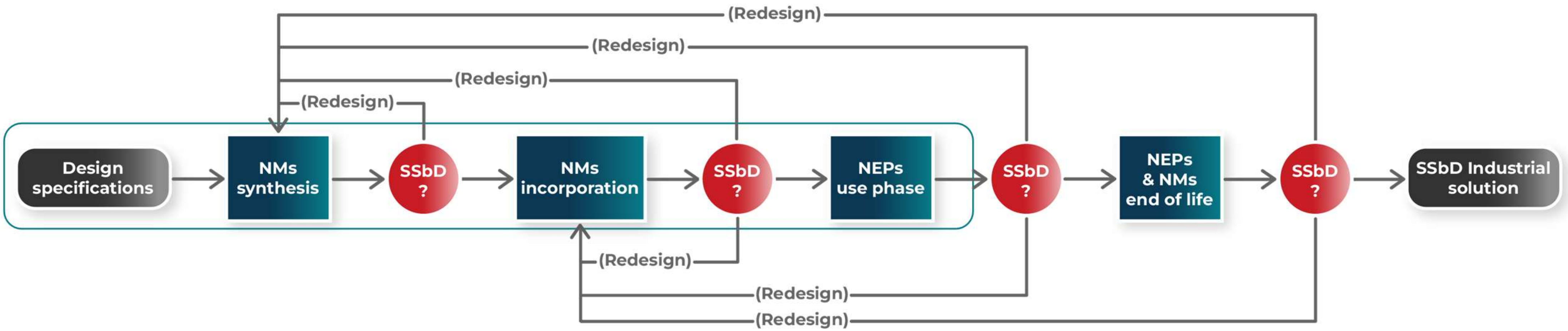
STAGE-GATE PROCESS FOR DESIGN & REDESIGN



Each LC may be treated separately through a **sequence of (sub-) case studies**

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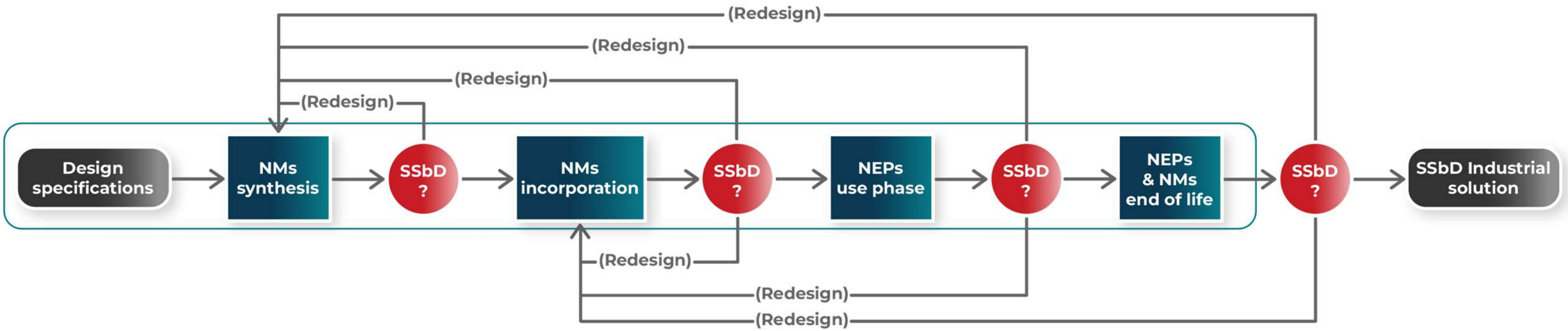
STAGE-GATE PROCESS FOR DESIGN & REDESIGN



Each LC may be treated separately through a **sequence of (sub-) case studies**

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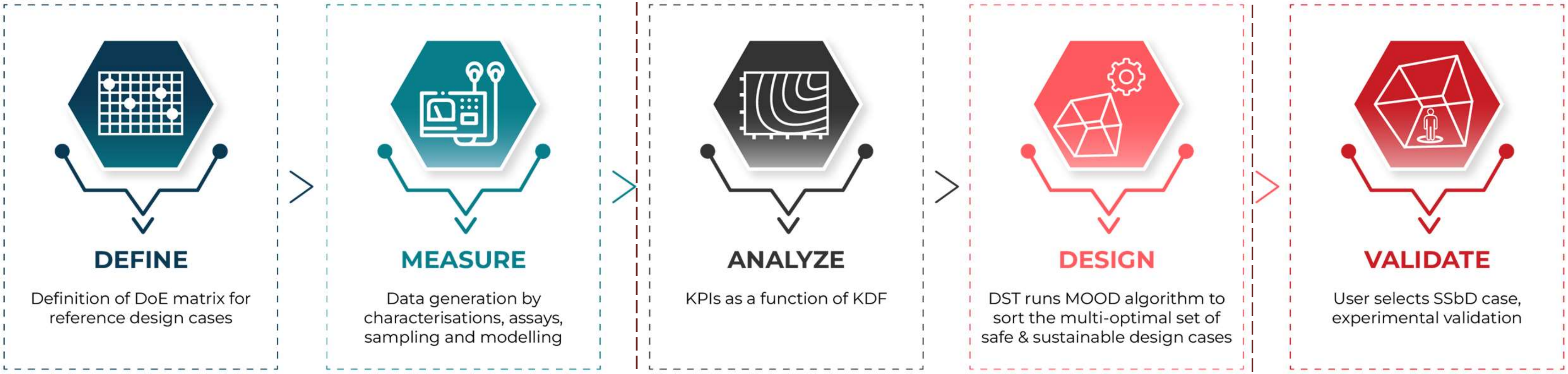
FROM DESIGN SPECIFICATIONS TO SOLUTION THROUGH D.M.A.D.V.

To reduce **time-to-market, costs,** use of **resources** and to reduce **implementation risks**



D.M.A.D.V. is a Six Sigma framework

MCDA

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THE SSBD ASSESSMENT METHODOLOGY IMPLEMENTATION FIVE ASSESSMENT PHASES

In compliance with JRC framework and inspired by ISO standards

I. **Goal and scope** definition (KDF, KPIs, DoEs, assumptions, system boundaries, LCs) (**DEFINE**)

II. **Data generation** by experimental work, modelling and Inventorying (**MEASURE**)

III. **impacts assessment** and multi-optimization to find set SSbD solutions (**ANALYZE**)

IV. **Interpretation** and humancentric decision making (Safe and Sustainable **DESIGN**).

MCDA

V. **VALIDATE** SSbD solution through generation of **samples** and **prototypes** to be assessed and tested

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Work and data flow

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DEFINING THE SSbD CASE STUDY

DEFINE

GOAL AND SCOPE

To be defined:
- The **reason** why we are performing LCA
- Intended audience actors & **stakeholders**
- The reference unit that we analyse ➔ called **FUNCTIONAL UNIT**
- The **system boundary** of the analysis
- Assumptions, exclusions and justification

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DEFINING THE SSbD CASE STUDY

DEFINE

GOAL AND SCOPE

FUNCTIONAL UNIT:
is a quantified description of the performance requirements that the **"product system"** fulfils.

- Product
- Process
- Service

Aspect
"**What**" (function(s) or service(s) provided)
"**How much**" (extent of the function or service provided)
"**How well**" (expected level of quality of the function or service)
"**How long**" (duration of the function or service/product lifetime)
"**Where**" (location/geography of the function or service)
"**For whom**" (beneficiary of the function or service)

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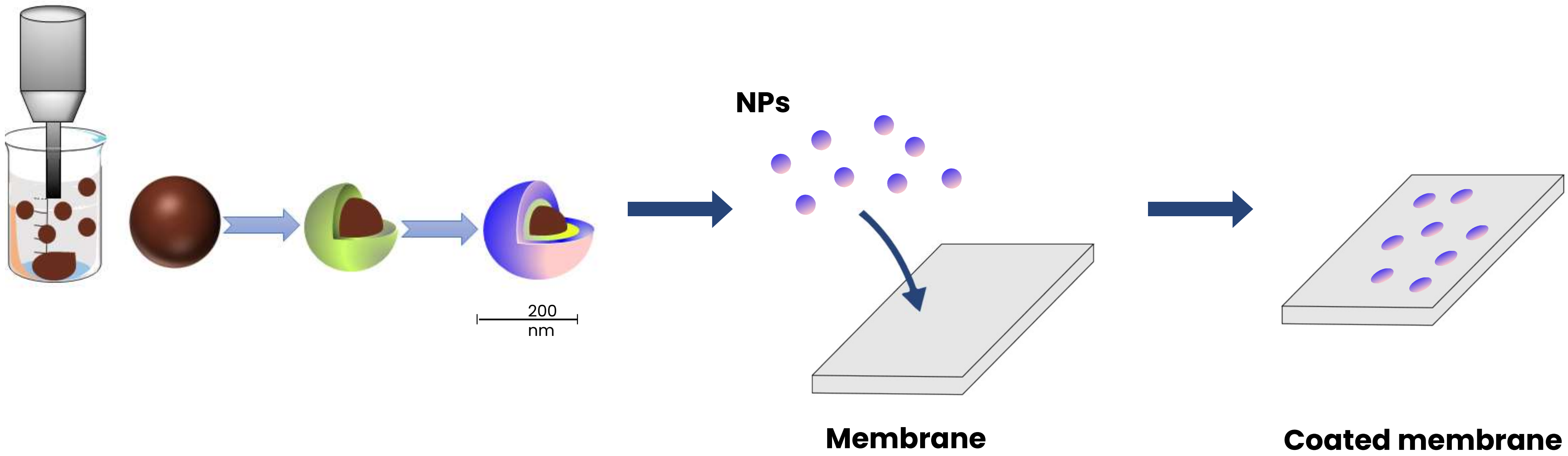
DEFINING THE SSbD CASE STUDY

DEFINE

THE SYSTEM AND ITS BOUNDARIES

Process scheme - Flow charts

(example: production of a water filtration membrane coated with NPs)



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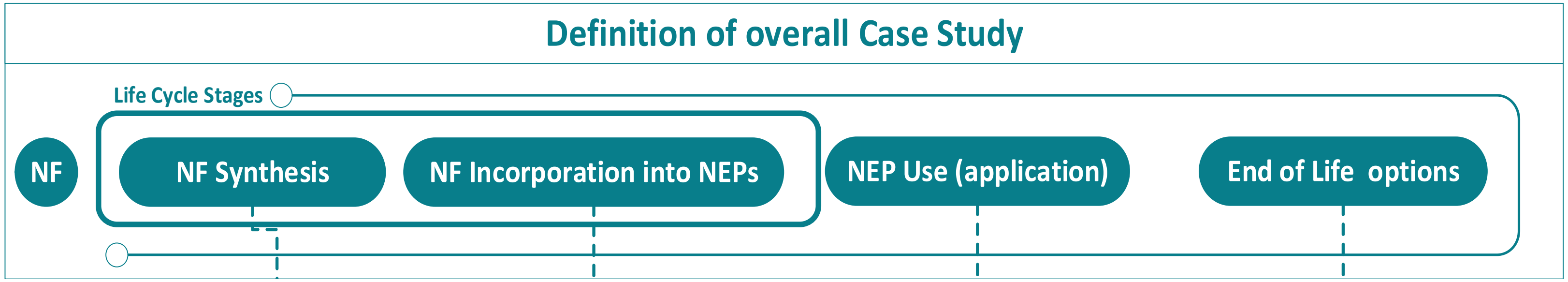
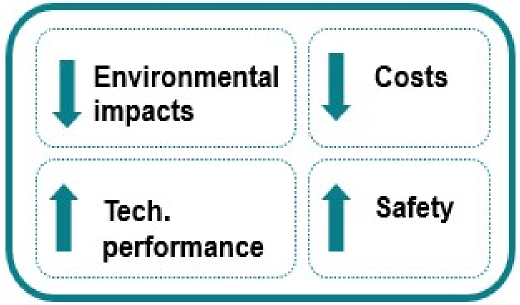
I) OVERALL CASE STUDY GOAL AND SCOPE





Case study	**Development of SSbD NEPs with antibacterial functionality**
Goal	Main objective: Redesign and efficient, effective safe and sustainable antimicrobial agent for textile applications: Specific objective: Identify the SSbD conditions for synthesis (LCS1) of NMs and incorporation (LCS2) of NMs that **simultaneously comply with** the following **design criteria** attainable through the design options: 1. e.g. NEP **antibacterial functionality** towards the following bacterial strains: E.Coli, S.Aureus 2. Minimize synthesis and incorporation process costs (**economic** sustainability) 3. Minimise Environmental impacts through LCS1 and LCS2(**Environment** sustainability) 4. Minimize human health risks associated to synthesis and incorporation process (**Safety**)

DEFINE

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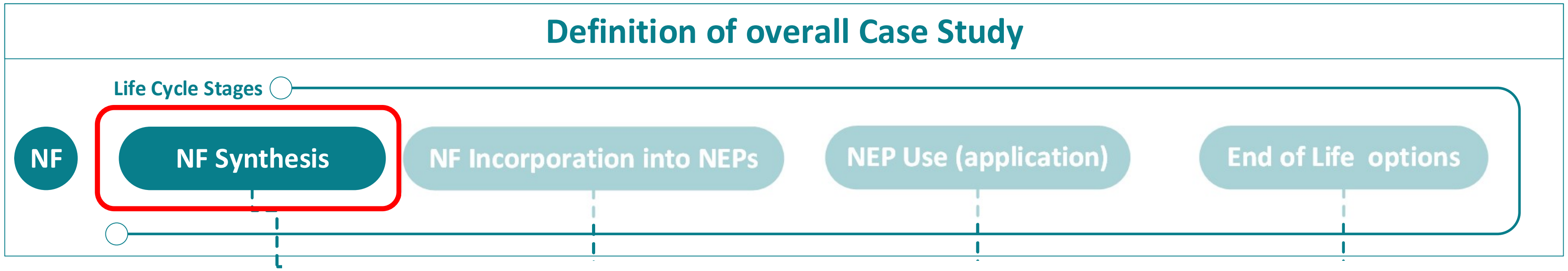
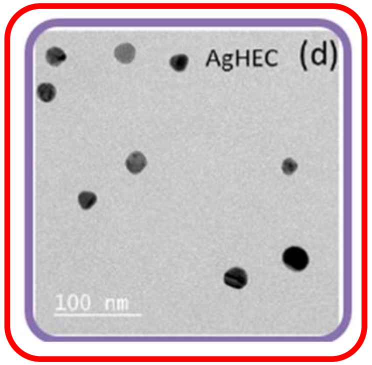
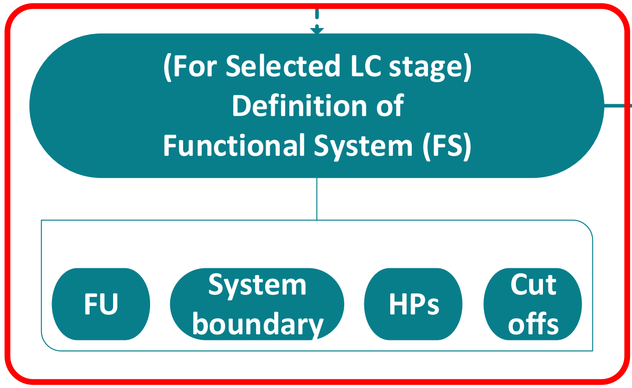
I) GOAL AND SCOPING

DEFINE







SCOPING	NM synthesis process
Scope	**LCS-1**: Analysis of the synthesis process in a "cradle to gate" approach.
FU	30mL of AgHEC hydrogel containing synthesized NF with AA>3
System	SolGel **synthesis** process
System Boundaries	from raw materials and energy sources to the NM samples "**from cradle to gate**"

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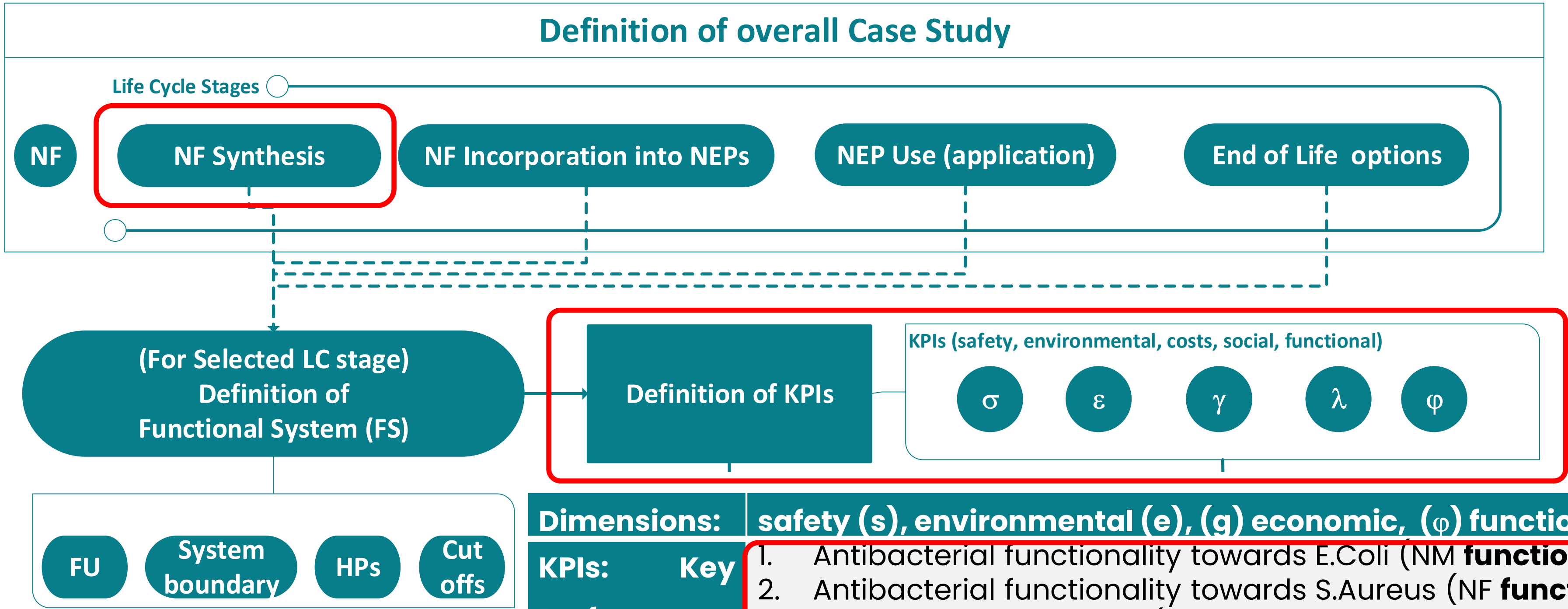
DEFINE

I) GOAL AND SCOPING: KPIs



Composite (derived) KPIs: cKPIs

cKPI1= ‹KPI1,KPI2›
cKPI2= =cKPI1/(KPI3*KPI4)

	NM Physic-chemical features
PCFs	PCF1: NM hydrodynamic diameter (nm) PCF2: Zeta potential (mV) PCF3: pH

Dimensions:	**safety (s), environmental (e), (g) economic, (φ) functional**
KPIs: Key Performance Indicators	1. Antibacterial functionality towards E.Coli (NM **functional** performance) 2. Antibacterial functionality towards S.Aureus (NF **functional** performance) 3. Synthesis process yield (Process **functional** performance) 4. Process costs (**economic** sustainability) 5. GWP- CO_2 emissions per unit synthesized NM (**Environment**) 6. HTTP- human toxicity potential associated to synthesis process (**Safety**)

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I) GOAL AND SCOPING: KDFs

(Key Performance Indicators KPIs and criteria)

DEFINE

Case study	AgHEC synthesis process: SCOPING
Measurement method of KPIs & PCFs	• Functionality assessment of **AA level**: log count reduction for 10mg/l concentration of hydrogel in bacterial culture (end-point assessment) • **LCC** of synthesis process including reagents and energy use • **LCA** for **global warming potential** assessment and **human toxicity potential** (mid-point assessment) **ISO 14040-44 standards** • Experimental Assessment of **process yields** • Experimental measurement **size** with TEM and **Zeta-potential** analyzer
Criteria / thresholds:	• **Maximization** of cKPI (<AA>/yeld/cost); cKPI=f(KPI-1, KPI-2, KPI-3, KPI-4) • **Minimization** of KPI-5 (environmental impact for global warming -**GWP**) • **Minimization** of KPI-6 (**toxicity** impact on humans)

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I) GOAL AND SCOPING: KDFs

(Key Decision Factors = design options)

DEFINE

Definition of overall Case Study

Life Cycle Stages

NF | NF Synthesis | NF Incorporation into NEPs | NEP Use (application) | End of Life options

(For Selected LC stage) Definition of Functional System (FS)

FU | System boundary | HPs | Cut offs

Definition of KPIs

KPIs (safety, environmental, costs, social, functional)

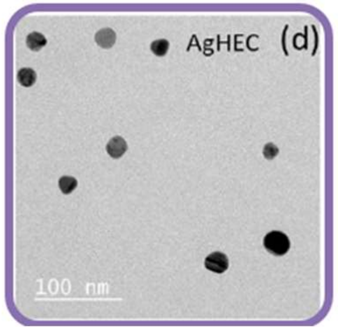
σ ε γ λ φ

Identification of Candidate Decision Factors (KDF)

Sensitivity analysis DoE screening

Human Experience

Selection of KDFs & KDFs values ranges



SCOPING:	NM synthesis process
KDFs : Key Decision Factors	KDF-1: Hydroxyethyl cellulose vs. Ag molar ratio (HEC/Ag, mol/mol). KDF-2: Sodium Hydroxide vs. Silver molar ratio (NaOH/Ag, mol/mol).

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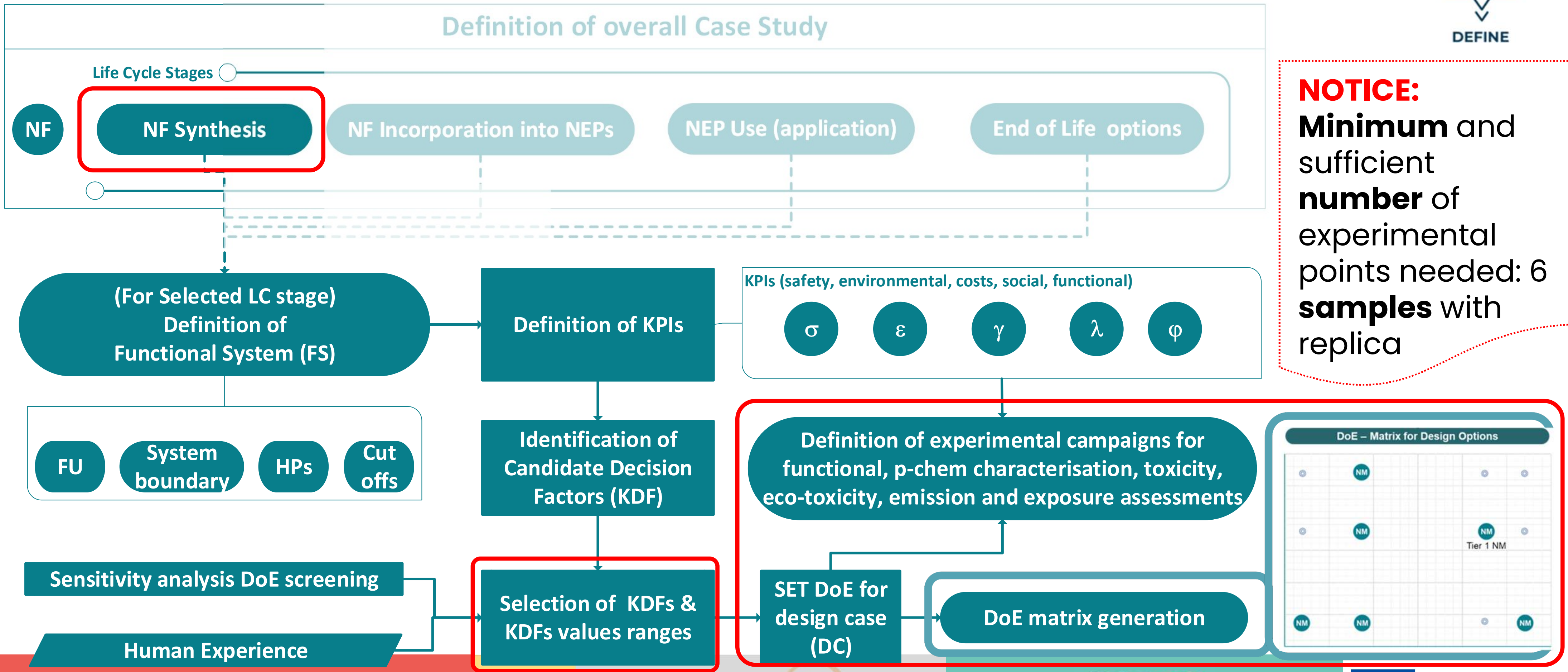
I) SCOPING: DESIGN OF EXPERIMENT – DOE: DECISION SPACE

DEFINE



NOTICE: **Minimum** and sufficient **number** of experimental points needed: 6 **samples** with replica

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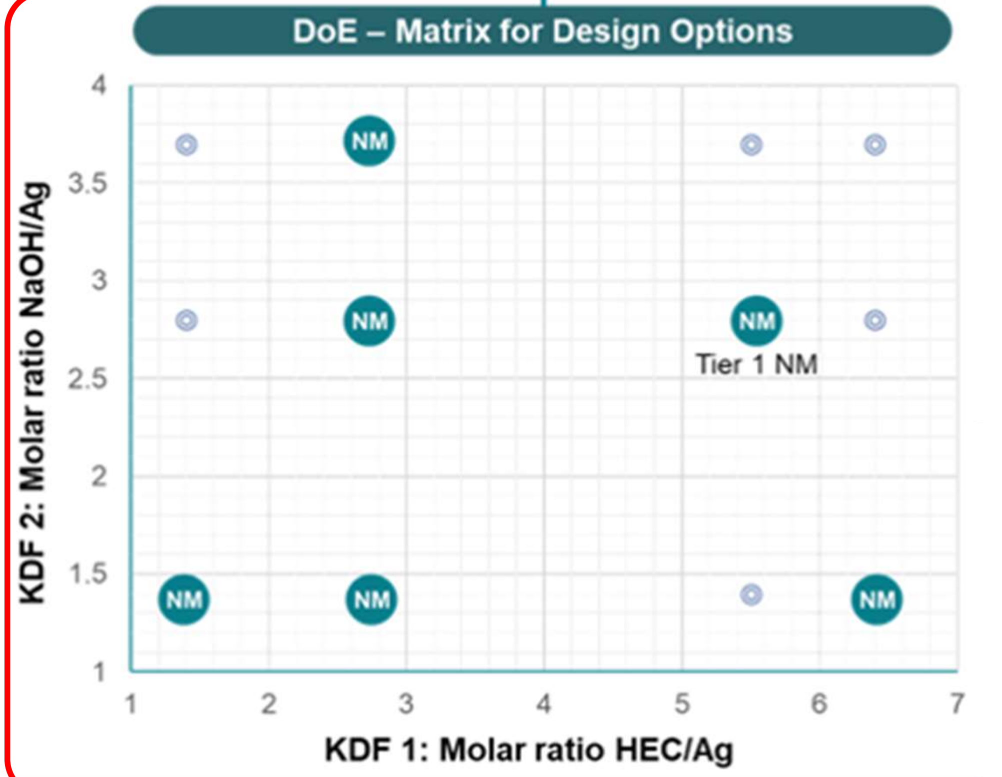
I) SCOPING: DESIGN OF EXPERIMENT – DOE: DECISION SPACE

DEFINE

Data points	HEC/Ag	NaOH/Ag
Point 1	2.8	1.4
Point 2	6.4	1.4
Point 3	6.4	3.7
Point 4	2.8	3.7
Point 5	5.5	2.8
Point 6	2.8	2.8

Minimum number of different syntheses processes (N=6) to assess (cost, environmental impacts) ⇔ generating a set of N=6 different samples (with replica) to characterise and test



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KDFs & KPIs

DEFINE

KPIs and KDFs may be discrete or continuous

KDF / KPIs	Discrete	continuous
discrete	dicrete / discrete	Discrete / continuous
continuous	continuous / discrete	Continous / contonuous

Example of discrete KDF: a set of candidate materials to be incorporated
Example of continuous KDF: amount of reagent, process temperature, process duration,..

Example of discrete KPI: upper/below cost threshold; scoring for functionality level (bad, sufficient, good, excellent)…
Example of continuous KPI: kg of CO_2 emitted in the synthesis, antibacterial level, …

Mixed discrete-continuous situations may occur, according to the case study

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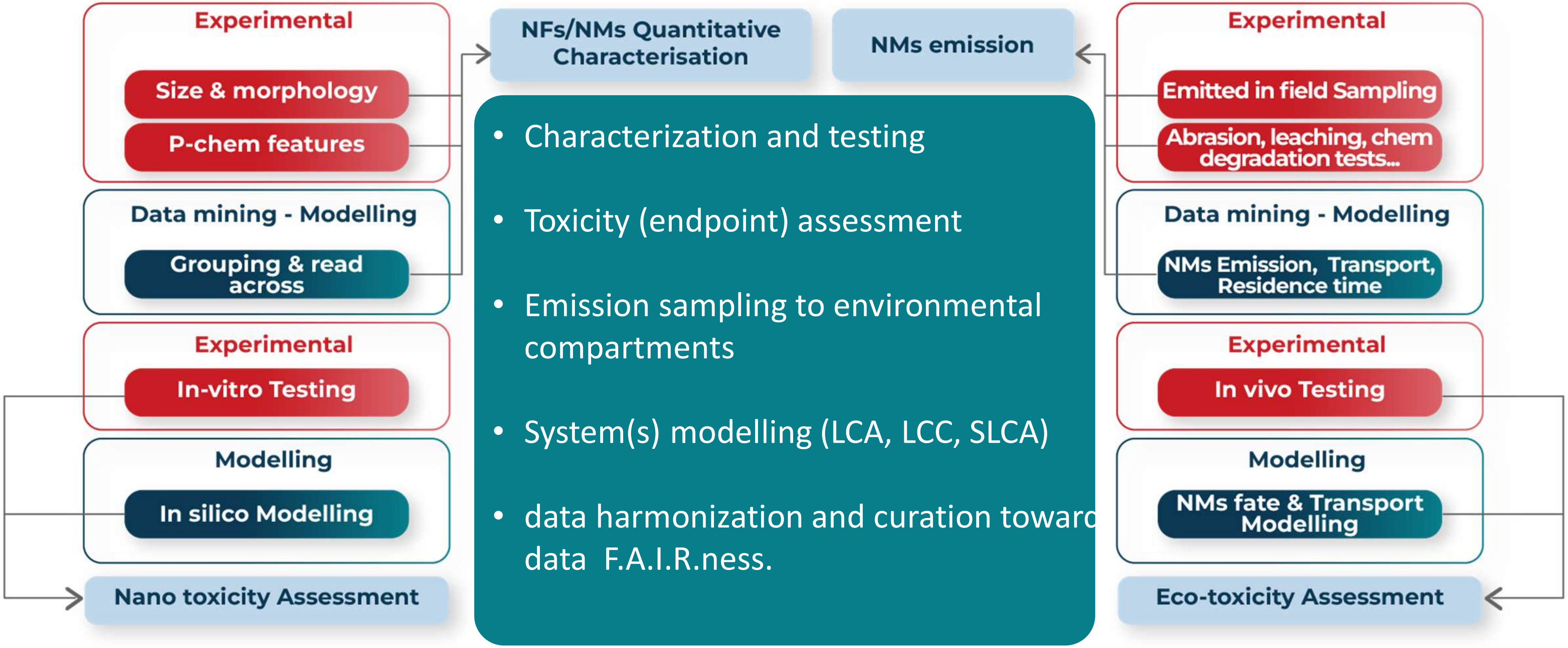
II) DATA GENERATION: EXPERIMENTAL AND MODELLING DATA INVENTORYING

MEASURE



- Characterization and testing
- Toxicity (endpoint) assessment
- Emission sampling to environmental compartments
- System(s) modelling (LCA, LCC, SLCA)
- data harmonization and curation toward data F.A.I.R.ness.

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MEASURE

II) DATA GENERATION: EXPERIMENTAL AND MODELLING DATA INVENTORYING

Multi-performance case specific generated DATA KPIs & PCFs

KDFs | **KPIs in environmental, economic, functional and safety dimensions + PCFs**

Envir. KPI | Econ. KPI | PCF (pChem) | Process | NFs Functional KPIs | Safety KPI

KDF-1	KDF-2	Environm. KPI	Econ. KPI	PCF	PCF	PCF	KPI	Antibacterial functionality		Antiviral functionality (against Beta variant)
HEC/Ag	NaOH/Ag	GWP100 (kg CO2 eq)	Total Cost (€)	Z-Pot (mV)	ØTEM (nm)	pH	↑Yield (%)	Antibacterial activity (E. coli) Conc Ag: 10 mg /l (↑)	Antibacterial activity (S. aureus) Conc Ag: 10 mg /l (↑)	Cytotoxicity CC50 (µg/ml) (↑)
2.8	1.4	0.0833	0.255	17.3	17	9.27	82.00	1.15	1.65	(-)
6.4	1.4	0.0863	0.318	20.1	13	9.58	100.00	4.08	3.53	6.0
6.4	3.7	0.0863	0.317	15.6	16	10.63	99.97	1.35	0.61	(-)
2.8	3.7	0.0834	0.255	11.3	18	10.80	99.97	1.85	1.48	(-)
5.5	2.8	0.0856	0.302	15.0	16	10.32	99.99	1.19	0.62	275.5
2.8	2.8	0.0834	0.255	12.3	18	10.51	100.00	1.82	0.43	191.3

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Multioptimisation towards SSbD decision making

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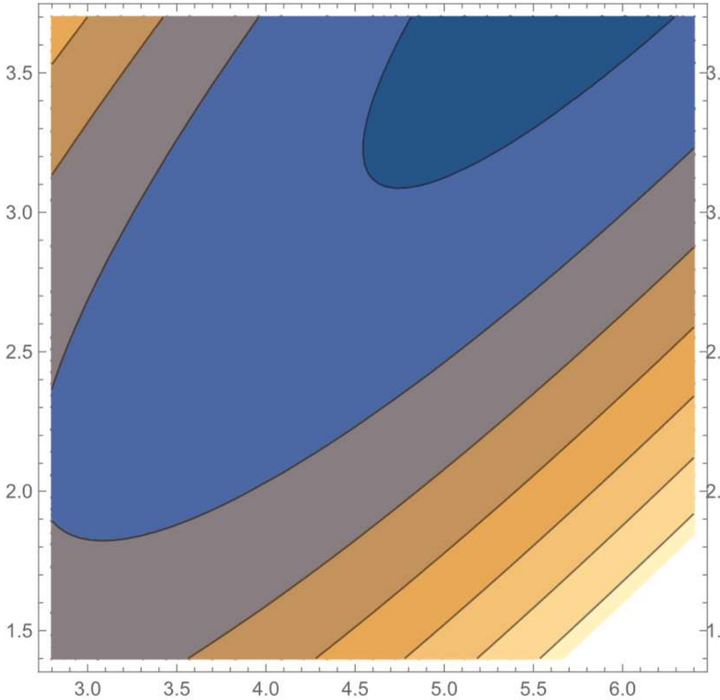
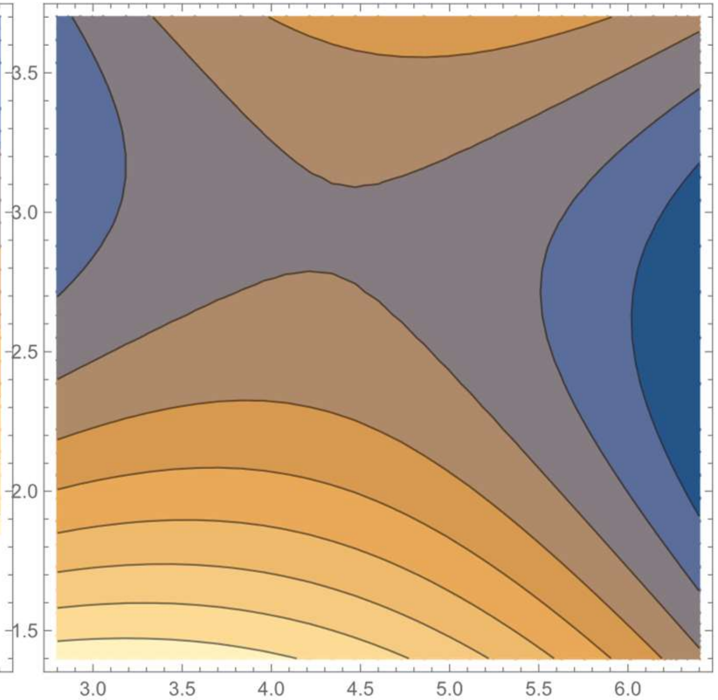
III) IMPACTS ASSESSMENT

ANALYZE

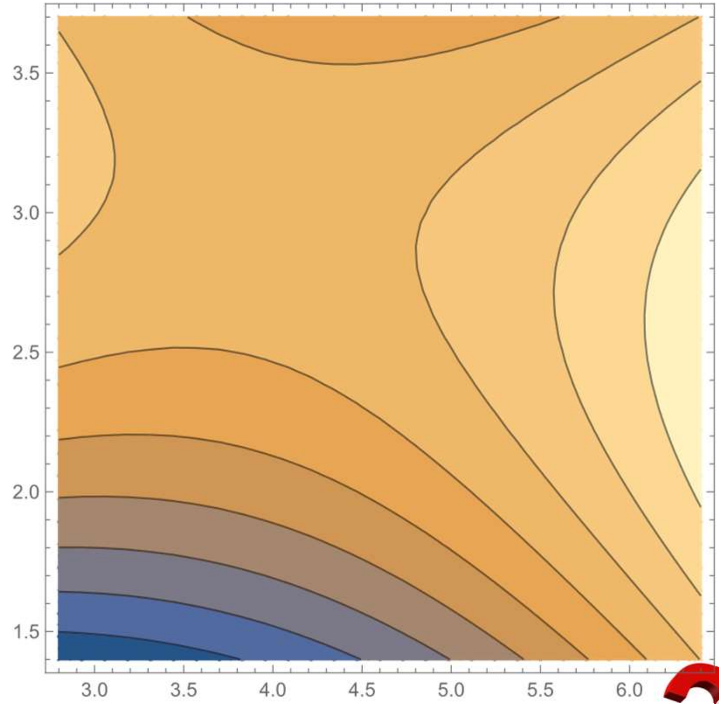
Multi AA Function/cost



Sustainability (GWP)



Safety (HTTP- mid point)



⇨ **MultiOptimisation: SSbD How to?**

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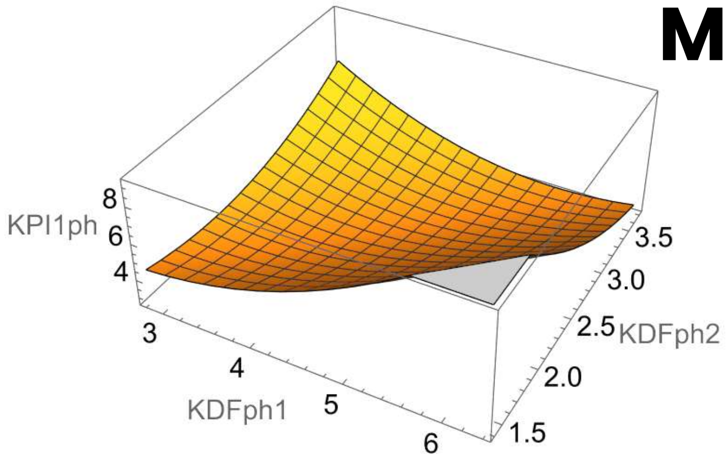
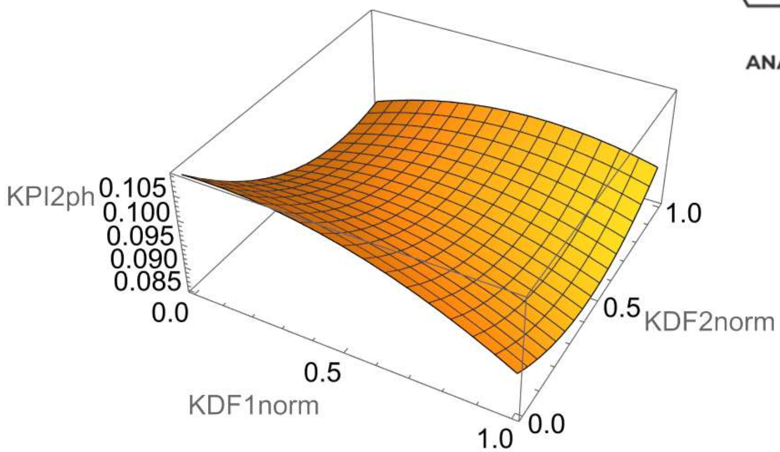
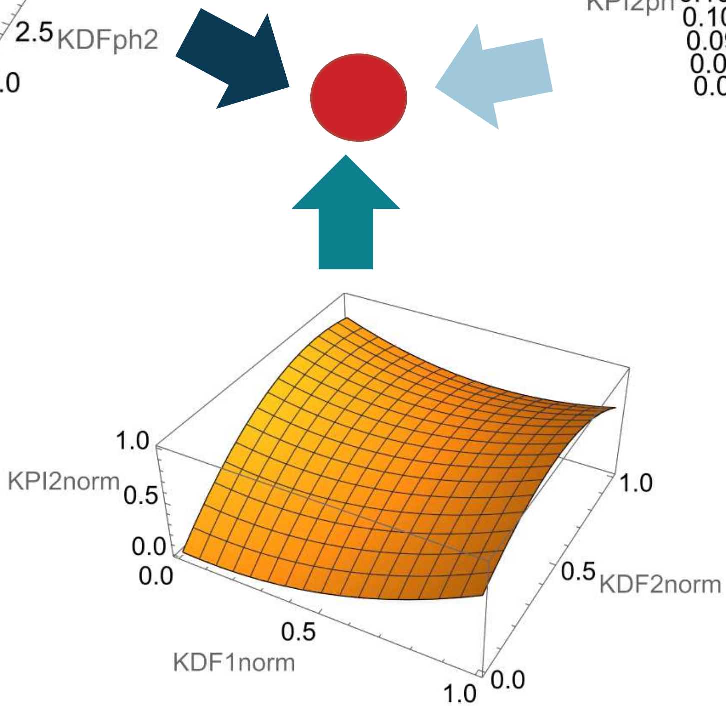
Multi space clashing!

ANALYZE







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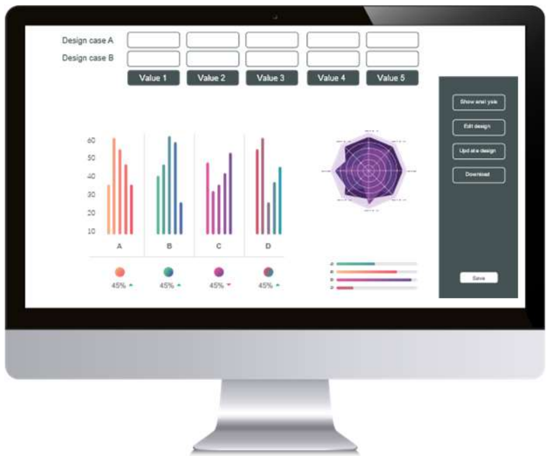
55

III) TOWARDS SSBD SOLUTIONS: MULTI-OPTIMIZATION

ANALYZE

MultiOptimal® 360



MultiOptimal360® is a Computation and Decision Support System (**DSS**) which enables:

- assessing the dependence of KPIs on KDFs
- the implementation of the Multi-Objective Optimization Design (**MOOD**) artificial intelligence (**AI**) **algorithm**
- **obtaining the set of (multi-optimal) SSbD cases**, simultaneously complying with safety, sustainability and functional KPIs requirements
- **Supporting humancentric decision** making

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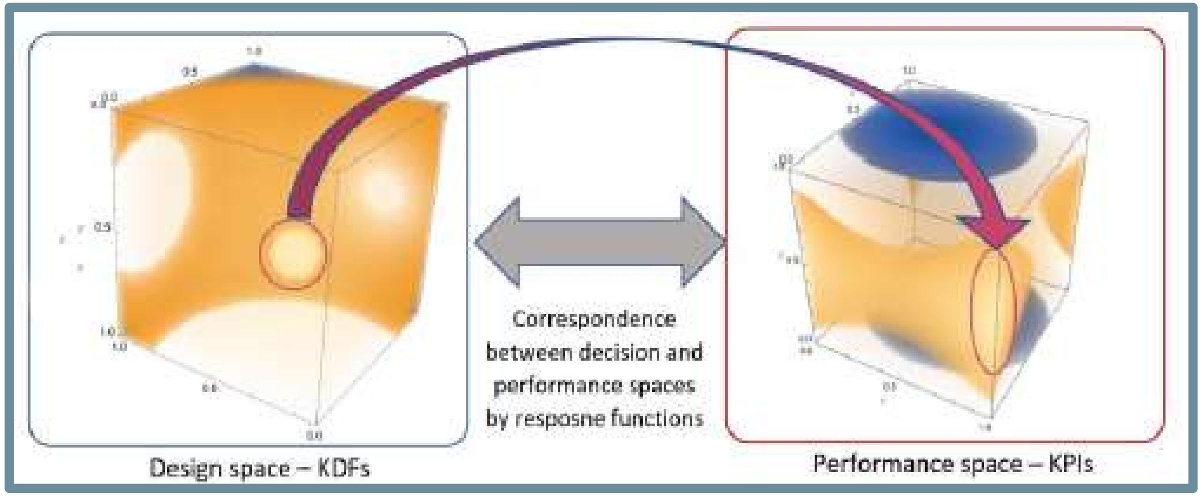
III) TOWARDS SSBD SOLUTIONS: IMPACTS ASSESSMENT & MULTI-OPTIMIZATION

ANALYZE



Design options

Corresponding performances

Generated data: KDFs, KPIs (phase ii)

DSS

KPIs Multi-Optimization (phase iii)

MultiOptimal® 360

Multi-Objective Optimization Design (MOOD)

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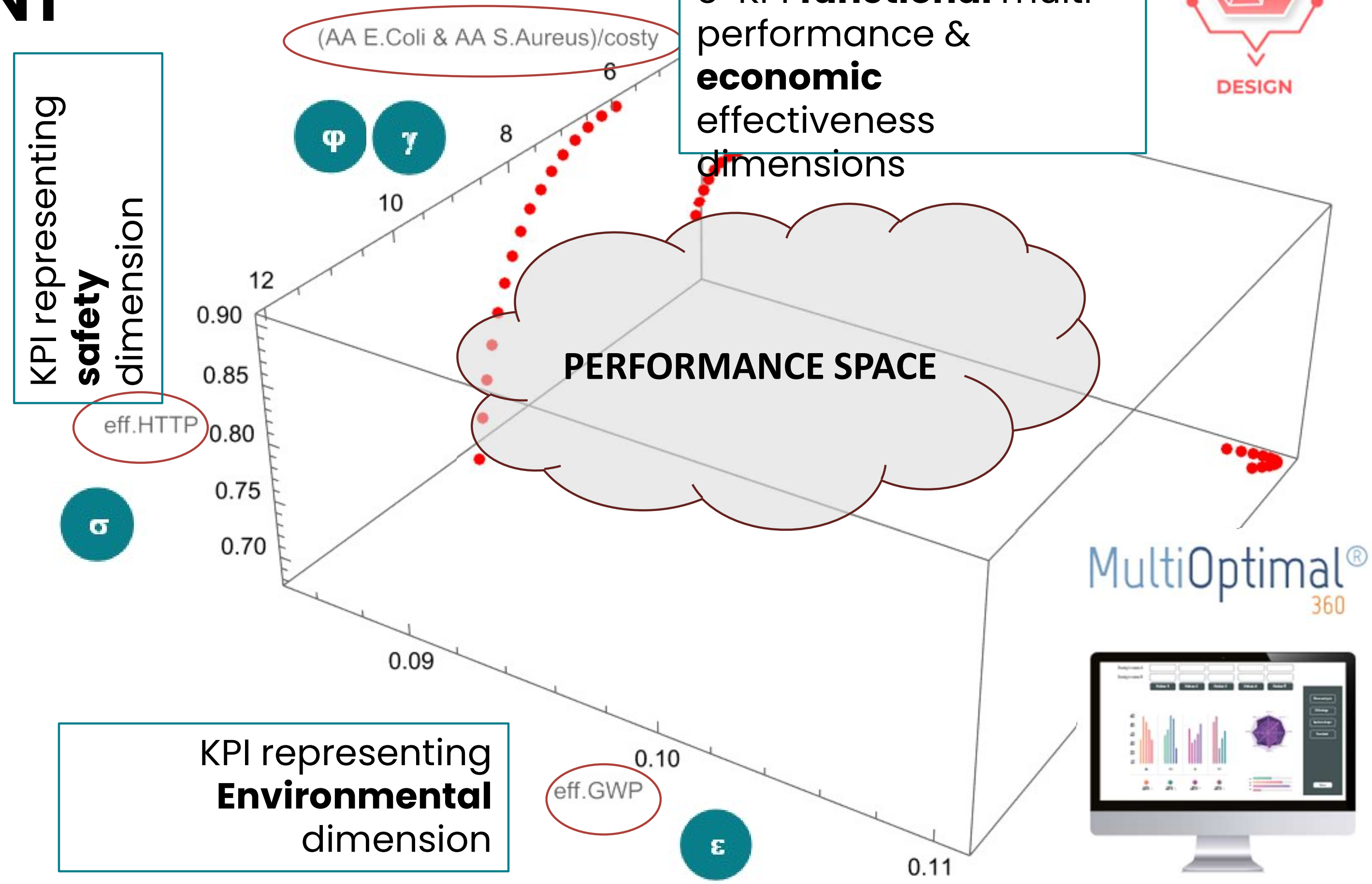
IV) DESIGN FOR SAFER AND MORE SUSTAINABLE ANTIBACTERIAL AGENT

DESIGN

Set of
SSbD cases
⇔
multi-optimized
KPIs
based on different
selection criteria



MultiOptimal® 360

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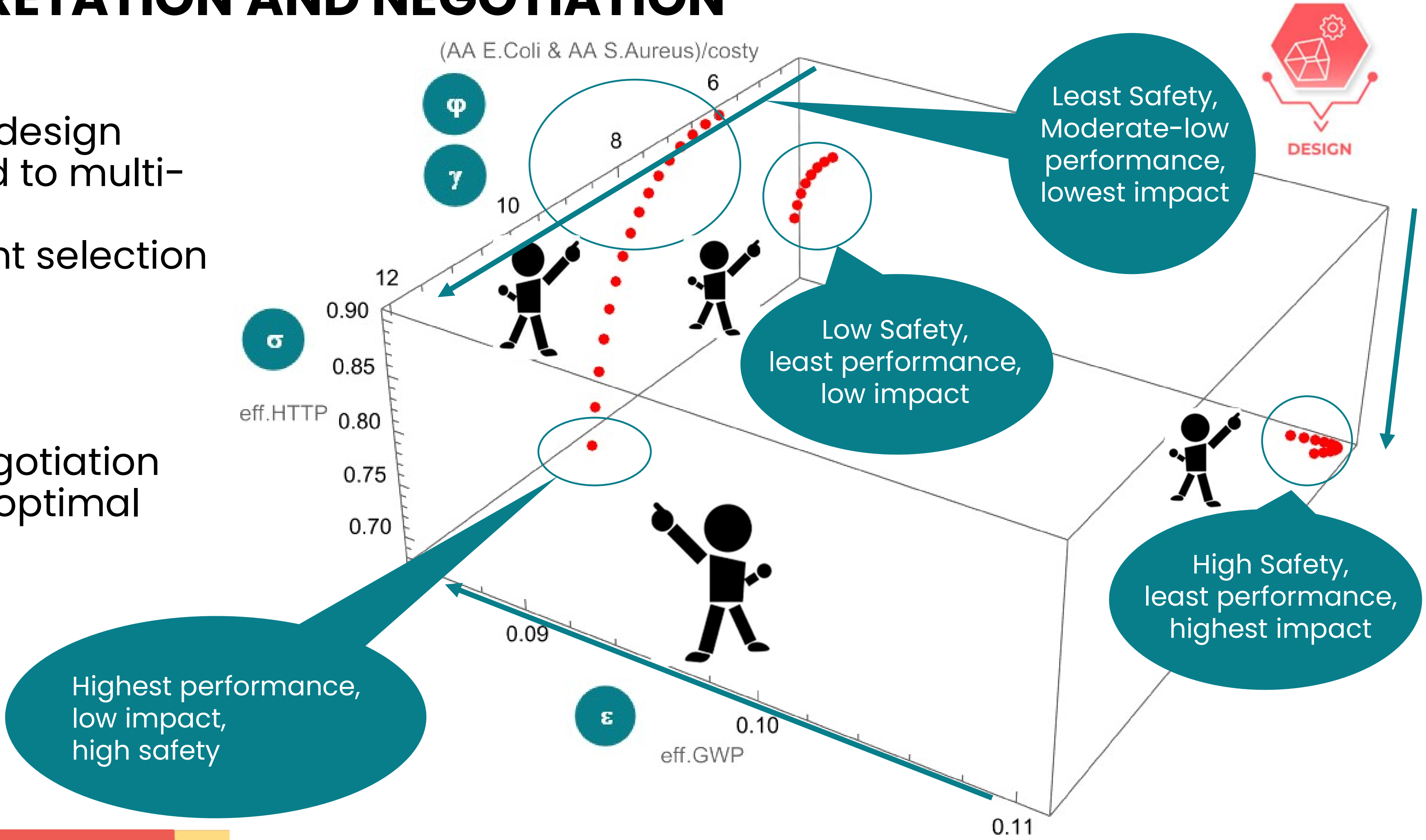
IV) INTERPRETATION AND NEGOTIATION

Interpretation of design cases associated to multi-optimized KPIs
based on different selection criteria

Stakeholders' negotiation based on multi-optimal design options



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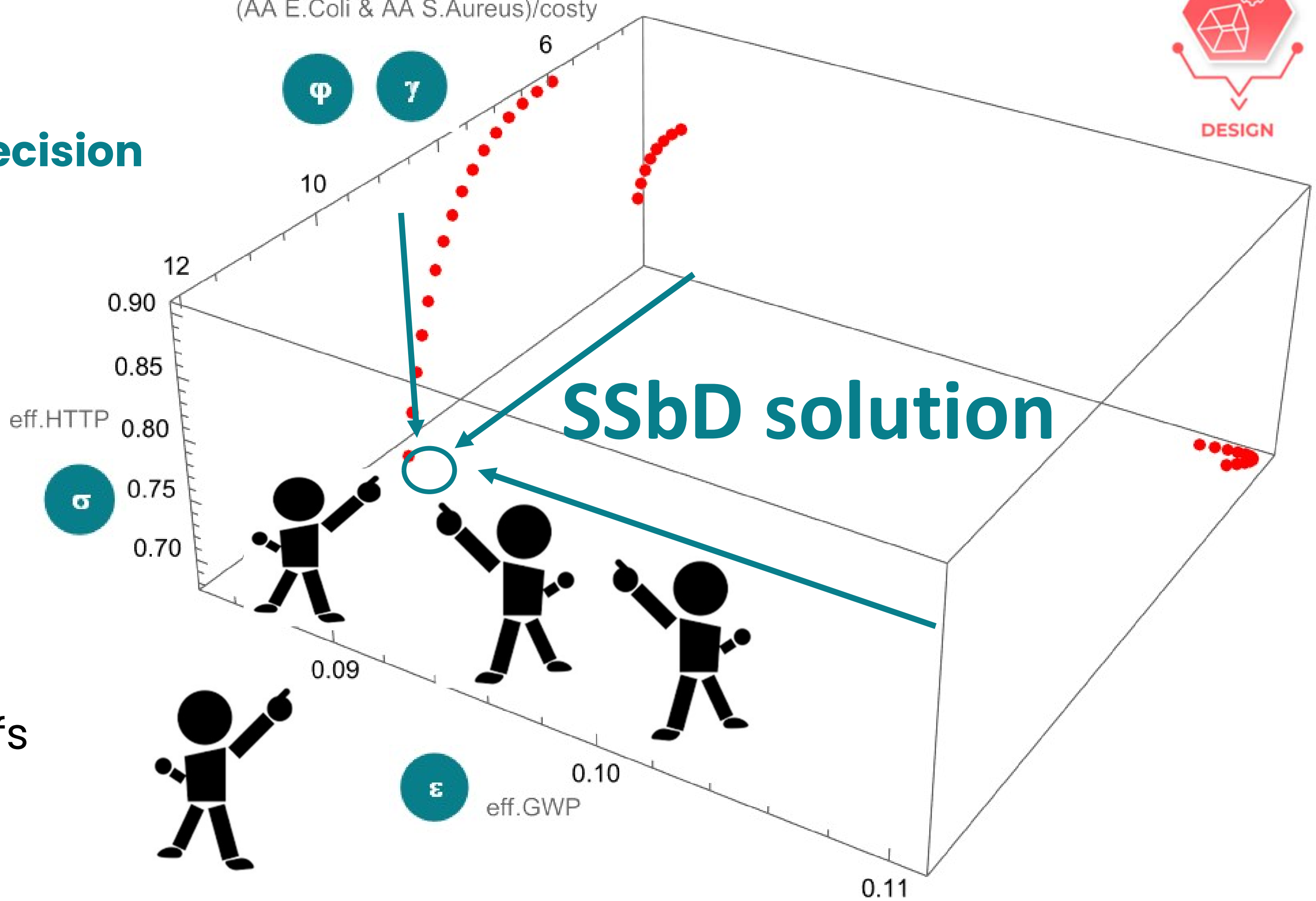
IV) INTERPRETATION AND SSBD SELECTION

humancentric informed decision making

- **SSbD set** ⇔ simplified scenario on attainable solutions based on BAT for basing consultations and experts' judgements
- **negotiation** to find tradeoffs and agreement on SSbD solution



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Take home messages

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TAKEAWAY MESSAGES

Characterizing features

i. **data driven** and **quantitative**
ii. **case-specific**
iii. **multilevel** & **stage-gate** for LCS assembly

Requirements

i. **Minimum** and sufficient **number** of **data points**
ii. **Harmonised datasets**
iii. Data covering **all** functional, environmental, socio-economic and safety **dimensions**

Research and Industrial sustainability and benefits of addressed SSbD methodology

i. **SSbD reduces the risk** of industrial R&D by **advanced assessment** the industrial and commercial exploitability of solutions (chemicals, advanced-/nano-materials, processes) (“*prevention is better than cure*”)
ii. **Minimum number** if experiments (tests, trials) ⇔ R&D **Reduced lead time (-60%)** & **Reduced costs (-80%)**
iii. MultiOptimal360™ (**DSS**) **enables** SSbD through Multi-Objective Optimization Design and supports **informed humancentric decisions making** for SSbD solutions

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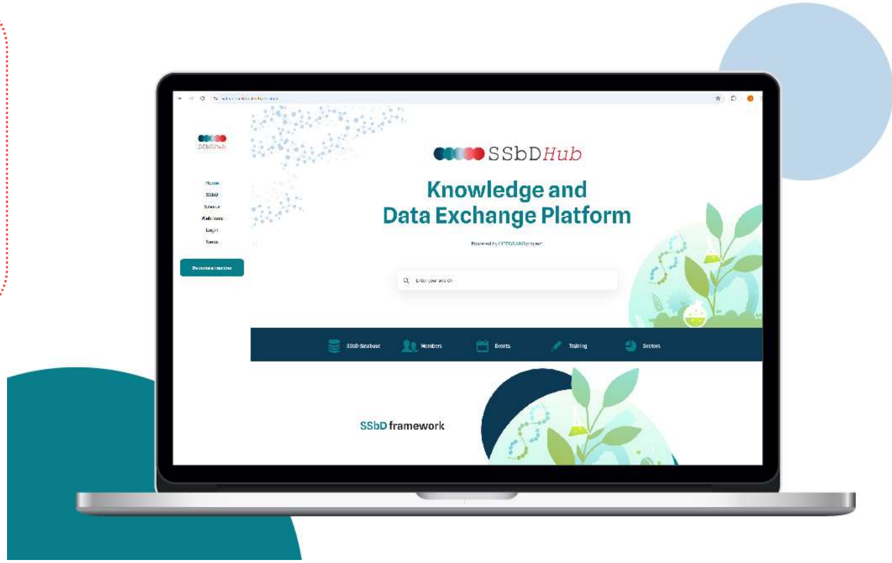
THE “SSBD HUB” PLATFORM

Since July 2024 the platform is **online!** SSbD Hub serves as an **interactive** website and is the main tool for communicating on **project initiatives.**



www.safeandsustainablebydesign.eu

Free contents:

- Webinars
- Workshops
- Literature

You are invited to **become members** and **register** on the platform, to benefit exclusive content.

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PROJECT HUB360 20th ANNIVERSARY 2005-2025

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Speaker: Massimo Perucca
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