Bridging AI and Sustainability: Advancing Safe and Sustainable by Design (SSbD) for Next-Gen Coating Materials

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Introduction

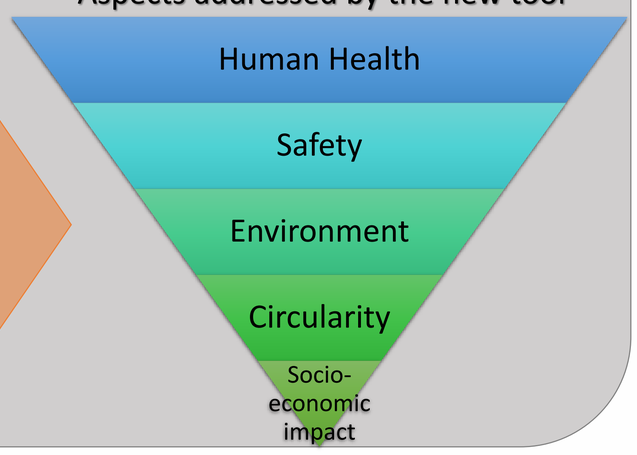
Multi-component HEA & HEC Coatings

High Entropy Alloys (HEAs) are an emerging materials category very promising for coatings production (high entropy coatings-HECs), but also for their sustainability performance throughout their entire lifecycle. LCA integrated with the SSbD holistic approach and Machine Learning (ML), incorporates different sustainability aspects (safety, environmental and socio-economic), identifies hotspots at low technology readiness level (TRL) and also facilitates the decision making towards a green transition on materials sector.

Outstanding novel properties

- **Mechanical** (hardness, toughness)
- **Chemical** (resistance to oxidation, corrosion, adhesion)
- **Physical** (high thermal stability, low diffusion)
- **Tribological** (high wear resistance)
- **Green and sustainable** (free of toxic substances & critical element)

Aspects addressed by the new tool



Objectives

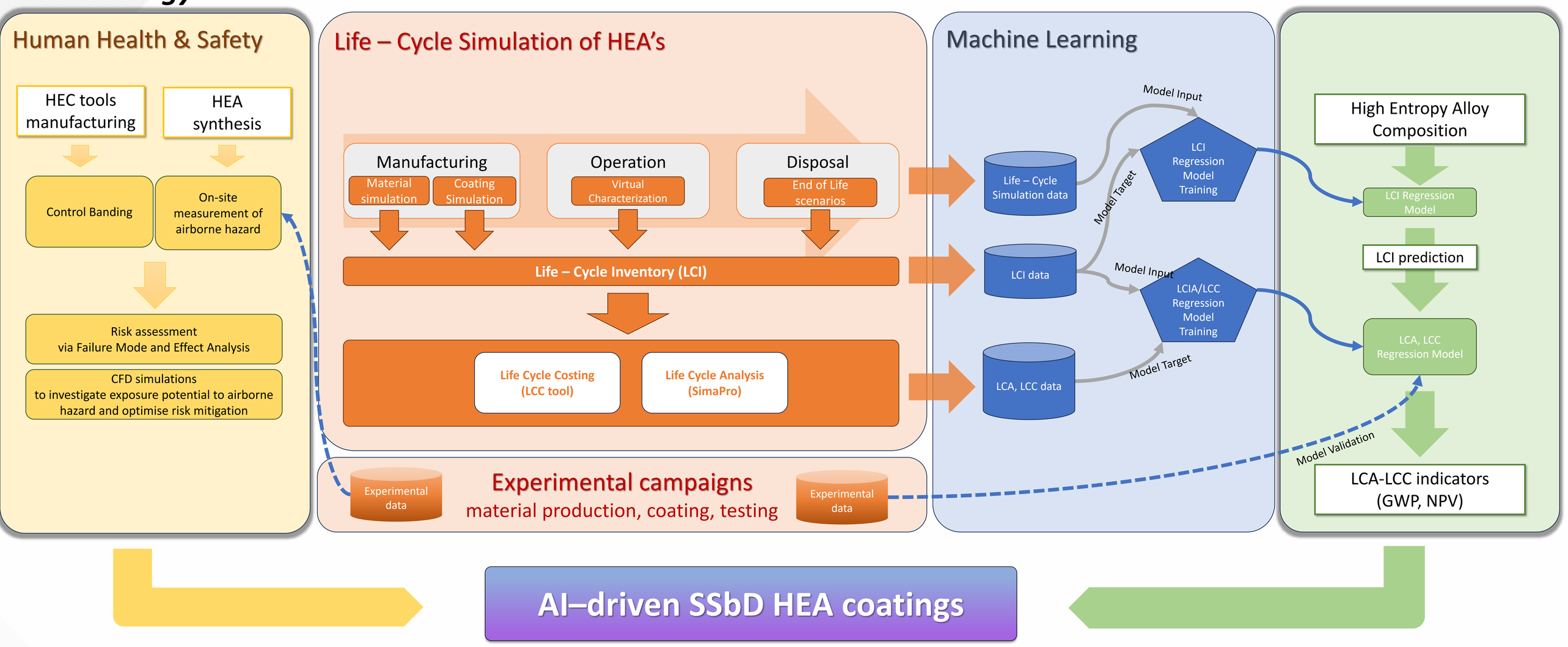
Reduced computational effort via rapid & high-quality data generation & LCIA/LCC calculations.

Visualization of results to promote immediate feedback. By varying different variables (identified as hotspots) the trend of results are presented in 3D plots

Rapid screening of different alternatives (incl. material & performance modelling) & **integrated uncertainty analysis**

Overall, the integration of ML in sustainability practices will **support informed decision making** from early design phase

Methodology



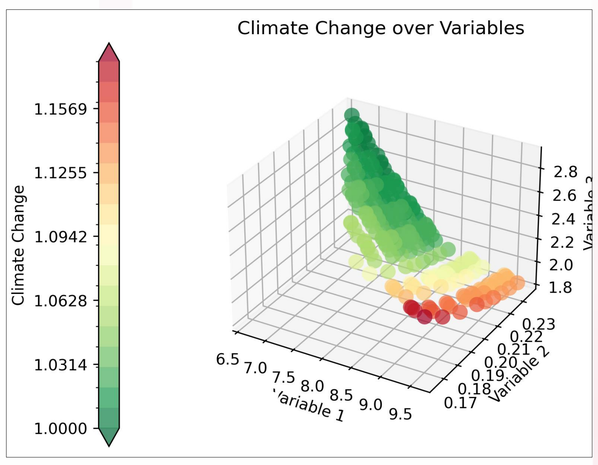
AI–driven SSbD HEA coatings

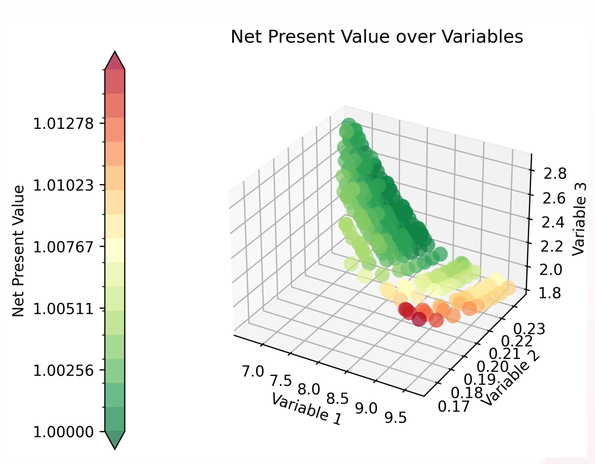
Expected Results

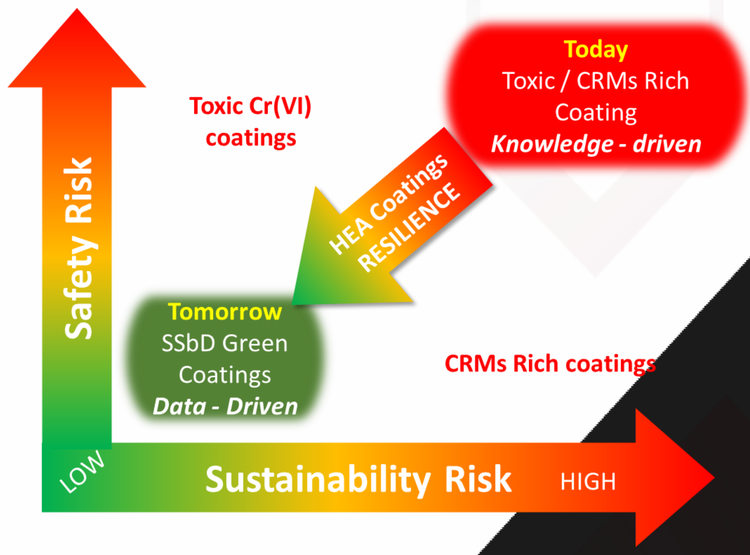
General Outcome

Indicative graphs for AI-driven Sustainability assessment for a set of optimized solutions

Climate Change & LCC Present Value vs. design parameter for all Life – Cycle phases







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