AI-driven multiscale methodology to develop Transparent Wood as sustainable functional material using SSbD

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1. Introduction

Efficient design, production, and optimization of new safe and sustainable materials for various industrial sectors is a future grand challenge for our society. Wood-based composite materials offer a solution and have therefore been the focus of experimental research and development for years. Computational materials design has the capacity to speed-up the development of these materials. However, this requires reliable models currently unavailable.

The project *'AI-driven multiscale methodology to develop Transparent Wood as sustainable functional material'* (AI-TranspWood), funded by the European Commission within the call HORIZON-CL4-2023-RESILIENCE-01-23, aims to create an Artificial Intelligence (AI)-driven multiscale methodology within the Safe and Sustainable by Design (SSbD) framework for functional wood-based composites. The concept will be demonstrated for Transparent Wood (TW), a promising material with potential applications in several industrial fields, such as construction, automotive, electronics and furniture.

Utilizing AI tools and conducting advanced experiments, we aim to create multiscale models spanning from the atomistic level to continuum scales. These models will address the manufacturing and mechanical aspects of transparent wood (TW) and facilitate virtual screening of bio-sourced alternatives to the chemicals used in TW production.

2. Transparent wood

Transparent wood (TW) acquired attention since its discovery and morphological characterization in 1992 by S. Fink [1]. Its complex microstructure originates from that of pristine wood, and the resulting composite is heterogeneous across the scales, providing interesting features: unlike wood, it is a lightweight, transparent to visible light, and, by the subsequent treatments (i.e., functionalization, modification, and infiltration with suitable resins) it becomes the best candidate for replacing glass and some plastics in a variety of applications.

European market for TW composites is new, and a recent report [2] estimates that global Transparent Wood industry will generate $208.1 million by 2031 witnessing a Compound

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Annual Growth Rate (CAGR) of 9.0% from 2022 to 2031, due to TW emerging as a promising alternative to petroleum-based harmful plastics [3]. Being eco-friendly, lighter, stronger, and having lower carbon footprint compared to traditional building materials it is expected to become a popular choice for energy-efficient buildings and sustainable construction projects.

3. AI-driven multiscale methodology

Computational modelling of TW properties requires specific physics-based modelling approaches spanning across several scales and physical domains. Such approaches are restricted by the computational power available, and the profound knowledge required.

AI-Transpwood proposes a systematic approach containing 17 work packages (WPs, Fig. 1) for complementing physics-based modelling and providing tractable software tools with the help of AI and ML (Fig. 2). It involves physics-based models developed in WPs 1, 2, and 4, used to create AI-based surrogate models (WP7). These surrogate models are then improved by integrating physics submodels directly into AI methodology (WP8). Finally, advanced physics models, such as non-linear finite element approaches, are linked to AI. The entire reality described by physics models is then connected to AI technology handling aspects not accommodated by physics-based models, e.g., geometric variability and material uncertainties due to growth and production irregularities.

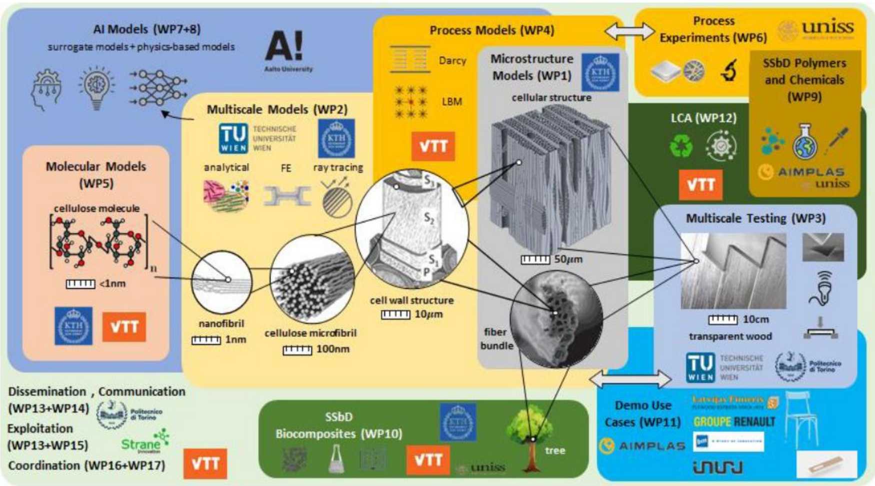

Figure 1: Structure of AI-TranspWood Project and associated WPs with leaders and main partners.

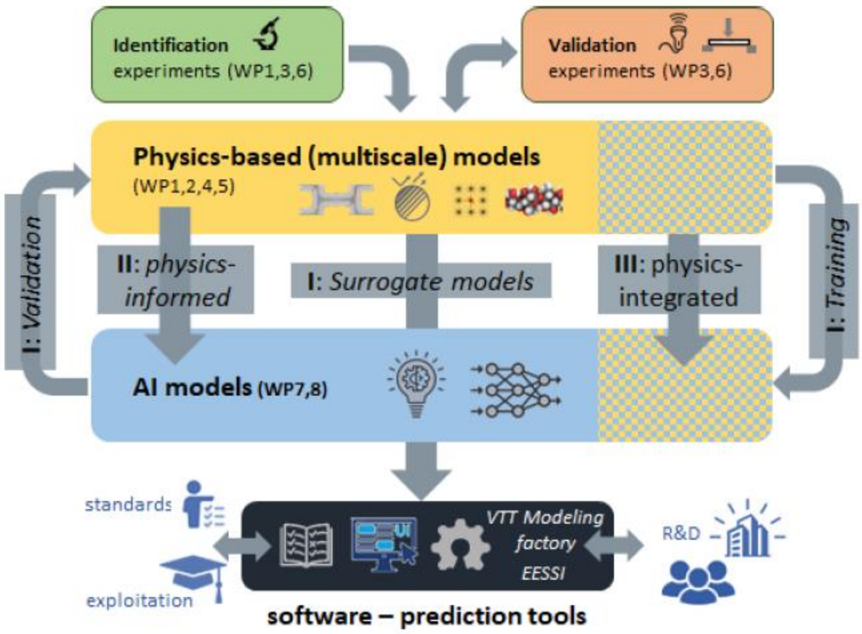

Figure 2: Conceptual three-stage process to link physics-based models to AI-methodology, and model classes which will then be implemented in predictive software.

4. Safe and Sustainable by Design concept

Safe and sustainable by design (SSbD) is a design approach where objectives such as minimizing hazardous chemicals use, reducing greenhouse gas emissions[2], and fostering materials reuse and recycling are built into product design. According to the call, "*the integration by computational modeling of the chemicals and materials functionality with the Safe and Sustainable by Design framework will have a key role in the green and digital transition of the European industry*", AI-TranspWood fully addresses this approach.

The AI-TranspWood project integrates efficiently advanced AI-driven computational models with the SSbD framework for wood-based composites and demonstrates the methodology for transparent wood (TW), with the vision to substitute substances of concerns such as plastic and glass in key applications. This will be possible thanks to the user-oriented design tools made available for industrial users.

In the project a formulation of safe and sustainable by design concept (SSbD) is defined for the purpose of screening polymers and chemicals selected for TW, and the final composites using data generated by models and eco-design or simplified LCA providing, identifying their safety and environmental and economic hot spots. The feedback from the screening study helps the material developers to improve the environmental performance at an early stage.

[2] https://ec.europa.eu/clima/eu-action/european-green-deal/2030-climate-target-plan_en

5. Models supporting design for lifecycle

After screening polymers, chemicals, wood and plant-based composites, SSbD formulation continues towards assessment of environmental impacts. This supports understanding of the sustainability of the whole service life of the selected materials and new transparent wood (TW) products to be developed. Finally, SSbD guidelines support the safe and sustainable design of use cases.

Environmental impacts are evaluated with data and knowledge gained during the project. The LCA and environmental footprint methodology will consider the whole value chain of the production system to quantify environmental impacts. Also, circularity and R-strategies of selected polymers and chemicals and biocomposites will be evaluated.

For supporting lifecycle of the products, the recycling of TW products will also be studied. Due to environmental and economic issues, mechanical recycling will be prioritized. However, due to the composition and nature of the polymers, chemical recycling will be required.

6. Conclusions

The aim of the project is to develop advanced TW through SSbD concept using AI-driven multiscale methodology. The communication between LCA and the material surrogate models published on open platforms will be created.

By developing AI-supported SSbD framework for TW, we contribute to the European Green Deal by providing innovative sustainable materials and cost-effective tools for European industries, paving the way towards green and sustainable transition. SSbD tools used by the chemicals and materials community with new transparent wood materials will increase the innovation capacity of SMEs and industry for future sustainable products.

7. References

[1] Fink, S. Transparent Wood—A New Approach in the Functional Study of Wood Structure. Holzforschung 1992, 46, 403–408.

[2] Transparent Wood Market by Application (Construction, Furniture, Solar Cell, Automotive Windshields, Packaging, Flexible Electronics, Others): Global Opportunity Analysis and Industry Forecast, 2021-2031. Report: A31788. www.alliedmarketresearch.com.
[3] https://www.alliedmarketresearch.com/transparent-wood-market-A31788

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