3D Simulation of Sustainable Porous Materials

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ABSTRACT

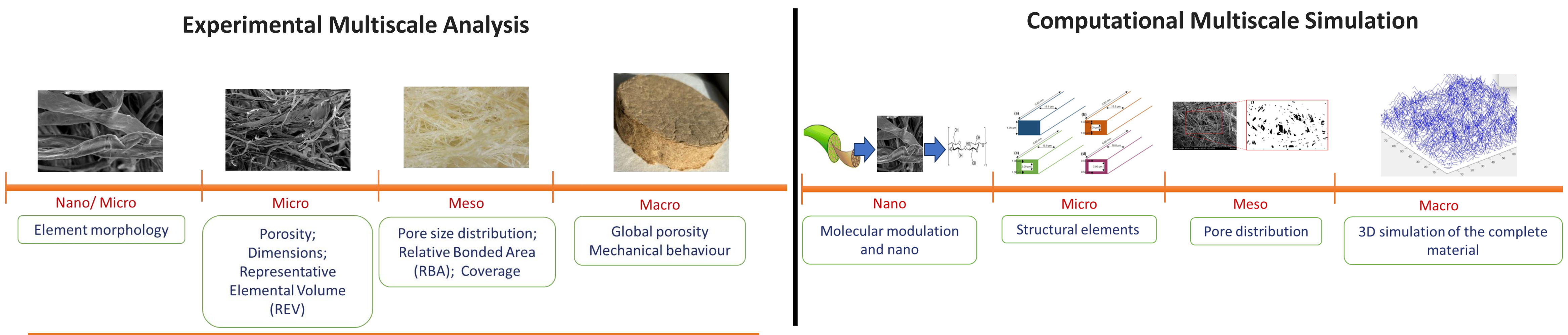
The progressive replacement of fossil-based materials towards sustainable materials made from recycled and renewable bioresources is aligned with the sustainability and circularity objectives.

The methodology presented combines the use of 3D simulation tools and experimental validation methodologies to optimize advanced porous structured materials

The results demonstrate that the 3D porosity and porous dimensions plays a decisive role in achieving the targeted performance properties. The findings show that materials exhibit a wide range of porosity values that directly influence their mechanical performance. A 3D multiscale methodology simulation approach supported by experimental data was implemented and validated.

The results indicate that the laboratory prototypes structures constitute an alternative to the conventional fossil-based systems existing in the market, but further optimization is needed.

MULTISCALE CHARACTERISATION



INTRODUCTION

- Fossil-based materials pose critical environmental challenges, driving the transition to sustainable alternatives aligned with circular economy principles.
- Cellulose stands out due to its abundance, biodegradability, and favourable mechanical performance. Porous cellulose structures are a promising replacement for fossil-based materials.
- Traditional experimental methods alone cannot capture the complexity of multiscale porous structures. 3D simulation enables prediction of material behaviour from structural parameters.

OBJECTIVES

- Combine 3D multiscale simulation tools with experimental validation to optimise cellulose-based porous materials.
- Evaluate the influence of porosity and pore dimensions on mechanical performance.
- Identify key structural parameters for further optimisation of sustainable formulations.

MATERIALS

Two commercial cellulose formulations:

- White Structure (WS) and Brown Structure (BS)
- Sodium dodecyl sulphate (SDS) – foaming agent
- Tannic acid – crosslinker

White Structure (WS)

Brown Structure (BS)

MANUFACTURING PROCESS

Reference Structures (RS):

- Cellulose fibres dispersed in water by mechanical stirring; filtered (ISO standard); air dried or dried in a convection oven; conditioned at 22 °C / 50% RH.

Porous Structures (PS):

- SDS and tannic acid introduced with high-shear mixing to induce porosity; cast into moulds; dried in convection oven; conditioned at 22 °C / 50% RH.

REFERENCES

[1] Curto et al., Mater. Wiss. Werkst. 42 (2011) 370–374 | [2] Morais et al., Polymers 13 (2021) 3982 | [3] Morais, Curto, BioResources 17 (2022) 4206–4225 | [4] Curto et al., Adv. Struct. Mater., Springer, 2015, pp. 301–321 | [5] Velosa, Curto, Mater. Wiss. Werkst. 56 (2025) 715–725 | [6] Morais, Curto, Heliyon 8 (2022) e09356

SEM IMAGING & POROSITY

- FEI Nova 200 SEM at 10 kV; magnifications 25× to 2000× for multiscale characterisation.
- Gravimetric porosity: $\rho_{app} = m / V$. Bulk porosity is a key parameter for experimental and simulation comparison.
- Image thresholding applied to SEM cross-sections to quantify pore count, area fraction, and mean perimeter.

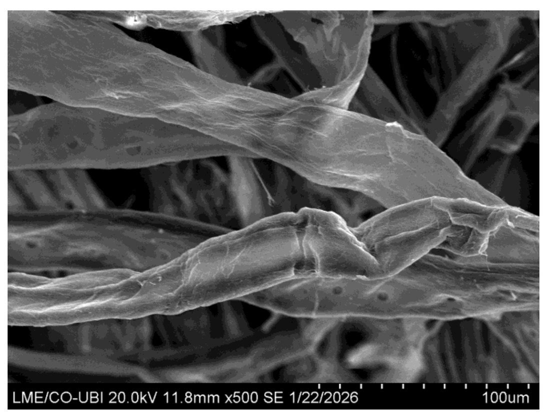


Fig. 1 – SEM images: BS (left) and WS (right) at 500×, 20 kV (FEI Nova 200)

FIBRE MORPHOLOGICAL ANALYSIS

- Automated analysis of 5,000–20,000 dispersed fibres per sample (Morfi system).
- Parameters: length, width, coarseness (linear weight), small particle content.

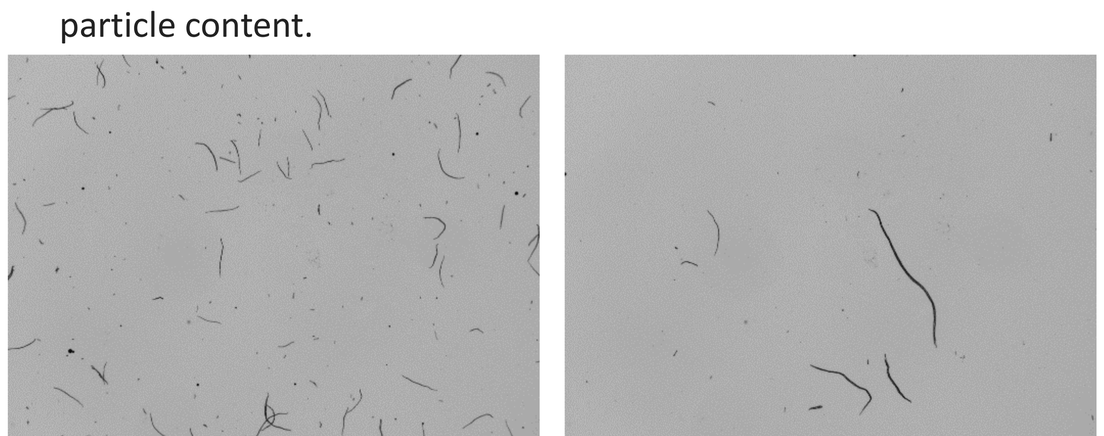


Fig. 3 – Morfi fibre microscopy: WS (left) and BS (right)

3D SIMULATION METHODOLOGY

- Voxel-based 3D Cartesian grid model implemented via cellular automata in MATLAB.
- Each voxel cell defined as solid or void. Mean pore diameter (d_{Pore}), voxel dimension, pore size distribution and total porosity (P) derived from experimental characterisation.
- Simulation outputs validated against laboratory-made structures.

RESULTS

Gravimetric Porosity

Porous structures (PS) reach up to 97.7% porosity vs. 88–91% for reference structures (RS):

- PS-White: 96.7% | PS-Brown: 97.7%
- RS-White: 88.8% | RS-Brown: 91.3%

SEM Porosity Analysis

- WS-PS: 130 pores, avg. area 83.0 px², fraction 7.5%
- BS-PS: 118 pores, avg. area 162.6 px², fraction 15.3%
- WS-RS: 112 pores, avg. area 79.9 px², fraction 9.0%
- BS-RS: 113 pores, avg. area 101.9 px², fraction 10.8%

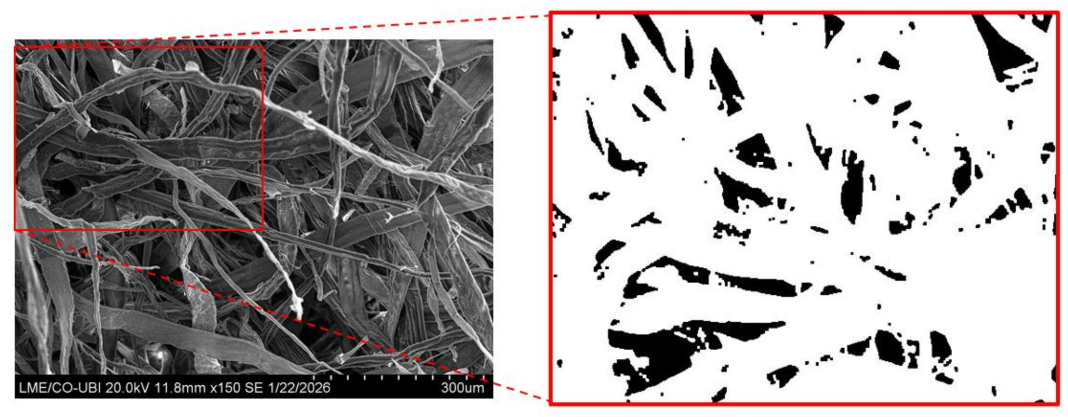


Fig. 2 – SEM + binary thresholding, WS porous structure

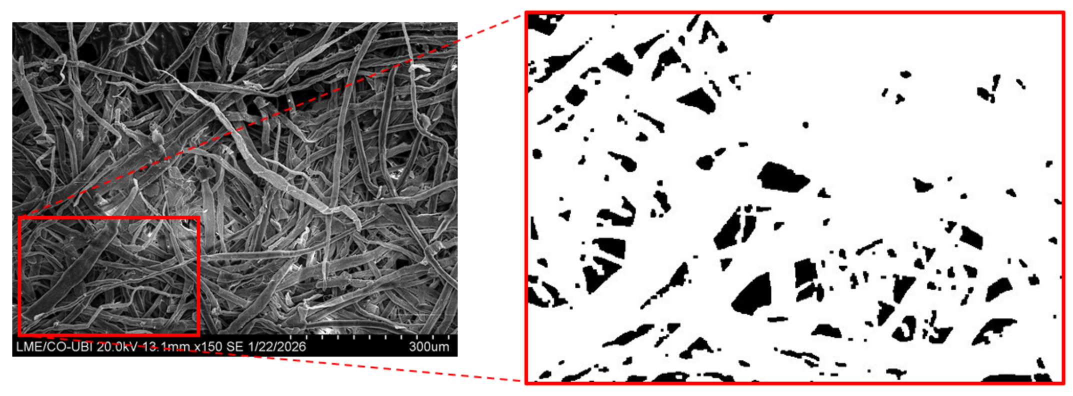


Fig. 3 – SEM + binary thresholding, BS porous structure

Fibre Morphology Results

- WS: 5,083 fibres | length 765.6 µm | width 16.3 µm | coarseness 0.11 mg/m
- BS: 5,012 fibres | length 1,510 µm | width 24.6 µm | coarseness 0.48 mg/m
- BS fibres are ~2× longer with higher coarseness, directly influencing the pore network topology.

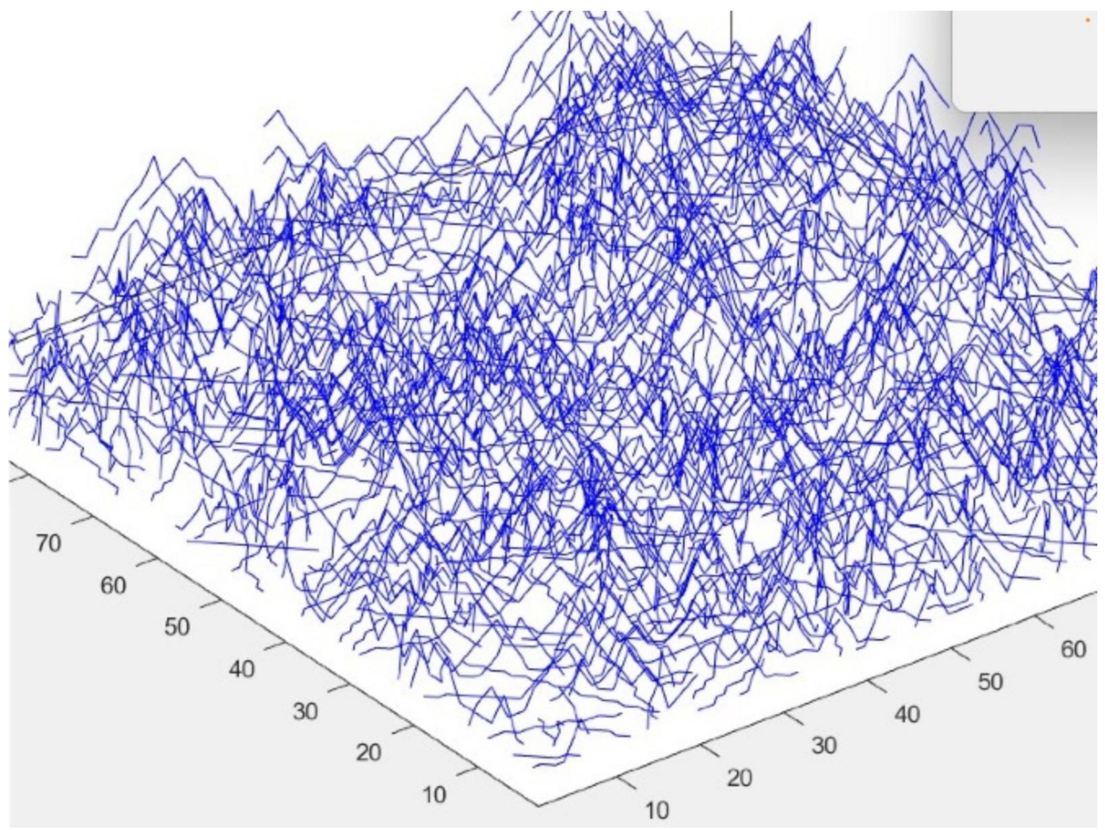


Fig. 4 – 3D voxel simulation output: virtual porous structure reconstruction

CONCLUSIONS

- 3D porosity and pore dimensions play a decisive role in achieving targeted performance properties.
- Materials exhibit a wide range of porosity values (88–98%) directly influencing mechanical performance.
- A 3D multiscale simulation methodology supported by experimental data was successfully implemented and validated.
- Laboratory prototype structures are a viable alternative to fossil-based systems; further optimisation is required.

ACKNOWLEDGEMENTS

This work was developed within the framework of the project Ecofoams- Fabrico Escalável de Ecoespumas de Isolamento reference CENTRO2030-FEDER-0211070 funded by COMPETE 2030, through Portugal 2030 and the European Union, carried out at the R&D Unit C-MAST, Faculty of Engineering, University of Beira Interior. Website: www.ecofoams.pt. The authors acknowledge the support granted by the Research Unit of the Centre for Mechanical and Aerospace Science and Technologies (C-MAST-UBI), through the Projects references UID/00151/2025 (https://doi.org/10.54499/UID/00151/2025), UID/PRR/00151/2025 (https://doi.org/10.54499/UID/PRR/00151/2025) and UID/PRR2/00151/2025 (https://doi.org/10.54499/UID/PRR2/00151/2025), funded by FCT - Fundação para a Ciência e a Tecnologia, IP/MECI. The authors are very grateful for the support granted by the Research Unit of Fiber Materials and Environmental Technologies (FibEnTech-UBI), through the Projects references UID/00195/2025 (https://doi.org/10.54499/UID/00195/2025), UID/PRR/00195/2025 (https://doi.org/10.54499/UID/PRR/00195/2025) and UID/PRR2/00195/2025 (https://doi.org/10.54499/UID/PRR2/00195/2025), funded by FCT - Fundação para a Ciência e a Tecnologia, IP/MECI. J. Nunes-Pereira also thanks FCT, for the contract under the Stimulus of Scientific Employment, Individual Support: 2022.05613.CEECIND (DOI: 10.54499/2022.05613.CEECIND/CP1746/CT0001). Veera Bhadraiah Sadhu acknowledges FCT - Fundação para a Ciência e a Tecnologia and University of Beira Interior for the research contract CEECINST/00016/2021/CP2828/CT0007 under the scope of the CEEC Institutional 2021, funded by FCT, and DOI 10.54499/CEECINST/00016/2021/CP2828/CT0007 (https://doi.org/10.54499/CEECINST/00016/2021/CP2828/CT0007). The authors are solely responsible for the content of this article, which does not reflect the opinion of the FCT.

29 JUNE - 3 JULY
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ACEX 229