

3D Simulation of Sustainable Porous Materials

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The accelerating need to replace fossil-based materials with sustainable alternatives has placed cellulose-based porous structures at the forefront of materials research. Conventional fossil-based foams impose serious environmental burdens that conflict with circular-economy objectives, while cellulose, owing to its natural abundance, biodegradability, and favourable mechanical properties, represents a compelling substitute. However, the complex, hierarchical pore architecture of cellulosic structures makes traditional experimental-only characterisation both time-consuming and incomplete, driving the need for computational tools that can model and predict material behaviour from structural parameters alone.

This work presents an integrated multiscale methodology that couples three-dimensional computational simulation with rigorous experimental characterisation to design, optimise, and validate sustainable porous cellulose materials. Two commercial cellulose formulations, white (WS) and brown (BS), were processed both as reference structures (RS), produced by standard filtration, and as porous structures (PS), cast from suspensions foamed with sodium dodecyl sulphate (SDS) and crosslinked with tannic acid. Automated fibre morphology analysis was conducted on more than 5,000 elements per sample, SEM imaging at magnifications ranging from 25x to 2,000x provided nano-to-meso pore data, and gravimetric measurements yielded bulk apparent density and porosity.

The 3D simulation was implemented as a voxel-based Cartesian grid model via cellular automata in MATLAB. Mean pore diameter, pore-size distribution, and total porosity derived from experimental characterisation were used as direct inputs to reconstruct the complete porous architecture virtually. Local weight and porosity gradients, pore-distribution maps, and structural parameters obtained from the simulation were then compared with laboratory measurements, confirming high predictive fidelity across all four sample types.

Gravimetric and SEM characterisation revealed a wide spread of structural properties across the four sample types. Reference structures displayed apparent densities of 154 kg/m³ (white) and 131 kg/m³ (brown), with porosities of 88.8% and 91.3% respectively. The introduction of SDS foaming and tannic acid crosslinking substantially altered both metrics: porous white structures reached a porosity of 96.7% at only 50 kg/m³, whilst porous brown structures attained 97.7% porosity at 35 kg/m³. Brown fibres, being longer (average 1,510 µm versus 766 µm) and coarser, also produced larger and more interconnected pores, as reflected in SEM-measured average pore areas roughly doubling those of their white counterparts. The 3D simulation reproduced these porosity gradients and pore-distribution maps with high fidelity across all sample types, confirming the predictive capability of the computational framework.

The laboratory prototype structures demonstrate clear potential as sustainable alternatives to fossil-based insulating systems. Further formulation optimisation, guided by the validated simulation platform, is expected to close the remaining performance gap.

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