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Temperature-driven surface reorganization in hot-pressed CTMP sheets revealed by ToF-SIMS and chemometrics

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ABSTRACT

The surface chemistry of bio-based materials governs surface properties such as adhesion but can also be central to other functional properties such as dry and wet strength; however, how temperature-driven reorganization during processing occurs is not well understood. Laboratory-prepared, statically hot-pressed CTMP handsheets and industrially hot-pressed CTMP sheets were investigated to evaluate temperature-dependent surface reorganization. A comparison of ATR-FTIR and ToF-SIMS results showed that heat treatment induced chemical changes at the nanometer scale. Principal component analysis revealed systematic variation with temperature and sheet side, while orthogonal partial least squares-discriminant analysis and a shared-and-unique-structures plot isolated temperature-specific marker ions independent of front/back-side asymmetry. At 100 °C, the front-side is enriched in small carbohydrate- and lignin-derived fragments, sterols, and medium-chain fatty acid salts; at 200 °C, lignin-derived fragments and long-chain fatty acids are more abundant. Side controls show no systematic front/back-side differences, indicating a primarily temperature-driven effect. The observed temperature-dependent surface reorganization is attributed to moisture-assisted thermal softening, enhanced polymer-segment mobility, and redistribution of lignin-rich domains and extractives during hot pressing. The marker-set workflow provides an interface-sensitive approach for resolving temperature-driven surface reorganization in chemically heterogeneous lignocellulosic materials.

1. Introduction

The chemical composition at the surface of bio-based materials is central to their functionality, yet our understanding of how their native macromolecules reorganize under thermal processing remains limited, partly because systematic methodologies for identifying surface-specific chemical changes are still scarce. Hot-pressing has been reported to enhance dry and wet strength of lignocellulosic fiber sheets [1,2], commonly attributed to thermally activated softening and redistribution of lignin that promotes interfacial contact and adhesion. Elevated temperatures may also drive migration of extractives and alter the balance between lignin- and carbohydrate-derived surface components [2,3], and thereby influence fiber–fiber joint strength [1,4].

While thermally induced surface migration has been demonstrated in related wood systems [5], surface-specific chemical changes during hot-pressing of CTMP sheets remain poorly resolved. Most existing studies emphasize bulk chemistry or macroscopic property changes, leaving the specific surface-active species that enrich or deplete during hot-pressing largely unresolved, despite their importance in controlling interfacial behavior during use [6]. A clearer understanding of these changes is essential for designing sustainable fiber materials that rely on inherent surface chemistry rather than on additional treatments.

Characterizing temperature-induced surface reorganization in lignocellulosic materials remains challenging because many conventional analytical techniques primarily probe bulk composition or provide limited molecular specificity at the outermost surface. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is particularly well suited for this purpose because it provides chemically resolved information from the outermost molecular layers while simultaneously detecting a broad range of organic and inorganic surface species.

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Techniques such as ATR-FTIR and X-ray photoelectron spectroscopy (XPS) can provide valuable complementary information on functional groups and elemental surface composition, respectively; however, they do not directly provide fragment-level molecular fingerprints from the outermost surface [7]. ToF-SIMS can resolve which ion families contribute to a surface-chemical contrast and how those signals are distributed across heterogeneous fiber surfaces [8]. However, the resulting spectra contain hundreds of fragment ions arising from lignocellulosic polymers, extractives, inorganic species, and their associated adducts. Consequently, multivariate chemometric methods are essential for extracting systematic chemical trends and identifying temperature-dependent surface fingerprints from these complex datasets [9,10].

2. Experimental

2.1. Materials

Chemi-thermomechanical pulp (CTMP) sheets were supplied by Stora Enso (Sweden). Unbleached softwood CTMP was dispersed in deionized water before being mixed at room temperature in an L&W pulp disintegrator (Lorentzen & Wettre, ABB) for 60,000 revolutions at 2900 rpm and formed into laboratory handsheets with a target grammage of 150 gm^{-2} were made according to the TAPPI/ANSI T 205 sp-18 standard41. Following sheet formation, the wet handsheets were dried under restraint between blotters with ~3 kg stainless-steel plate to produce flat and uniform sheets. The laboratory handsheets were subsequently subjected to static hot pressing using a LabPro press (Fontijne Presses, The Netherlands). The sheets (with a diameter of 16.5 cm) were placed between two metal plates lined with Teflon sheets and pressed at a constant force of 10 kN for 1 min. Three sample sets were prepared: a reference (25 °C), and hot-pressed sheets at 100 °C and 200 °C. After hot pressing, the sheets treated at elevated temperatures were immediately transferred to room temperature and allowed to cool prior to surface characterization.

Industrially hot-pressed CTMP sheets from Stora Enso were prepared as described previously [11] and subsequently hot-pressed at two temperatures (100 and 200 °C) under otherwise identical conditions (line load, nip pressure, and web speed). For each hot-pressing temperature, the side exposed to the heated surface is referred to as the front surface, whereas the opposite side is referred to as the back (reference) surface.

Detailed analytical procedures for determination of the chemical composition CTMP and results are provided in the Supporting Information (SI).

2.2. ToF-SIMS analysis

ToF-SIMS measurements were performed on both sides of the sheets prepared from the same batch at multiple surface locations, giving six independent spectra per side and temperature (n = 6 for all analyses, i.e., 100 °C front-side, 100 °C back-side, 200 °C front-side, and 200 °C back-side, where front-side means the side that was exposed to heat).

Surface chemical profiles were acquired by time-of-flight secondary ion mass spectrometry (ToF-SIMS V, IONTOF GmbH, Münster, Germany) operated in positive-ion mode with a pulsed Bi3+primary ion beam (25 keV, ~0.35 pA). Static SIMS conditions were maintained (primary ion dose $<1 \times 10^{13}$ ions cm^{-2}). Spectra were recorded over a 500 × 500 μm^2 raster with 15 scans per analysis position and a mass range of *m/z* 0-800 with the cycle time of 125 μs. Charge compensation was applied using a low-energy electron flood gun. For each sheet type and treatment (100 and 200 °C, front- and back-side), six independent surface locations were measured (n = 6), yielding a total of 24 spectra for multivariate analysis. Peak lists were generated in SurfaceLab, and single-ion intensities were normalized to the total ion current (TIC) prior to further data processing.

2.3. Multivariate analysis

Chemometric analysis was performed using SIMCA 18 (Sartorius/Umetrics, Umeå, Sweden). TIC-normalized peak intensities were mean-centered and Pareto-scaled before modelling [12]. Supervised orthogonal projections to latent structures discriminant analysis (OPLS-DA) models were built to compare (i) front- and back-sides at each hot-pressing temperature and (ii) 100 and 200 °C treatments for the hot-pressed front-side. Shared and unique structures (SUS) plots were constructed by plotting the *p(corr)* loadings from the temperature model against those from the corresponding side model. Model validity was assessed by cross-validation, CV-ANOVA ($p < 0.05$), and permutation testing. Marker ions were selected based on the combination of high absolute correlation | *p(corr)* | (typically ≥0.4-0.6), variable-importance-in-projection (VIP) ≥ 1.0, and statistically significant intensity differences according to Welch's unequal-variance *t*-test on TIC-normalized data ($p < 0.05$).

3. Results and discussion

3.1. ATR-FTIR and ToF-SIMS analysis of static hot-pressed laboratory sheets

To determine whether temperature-dependent chemical changes occur at the fiber surface (within ~1–2 μm), ATR-FTIR measurements were performed on laboratory-prepared CTMP handsheets on three sample classes (reference and hot-pressed sheets (100 °C and 200 °C)) [13]. The average IR spectra exhibited the characteristic lignocellulosic bands of cellulose, hemicelluloses, and lignin, with no pronounced differences between the three sample classes. Even using principal component analysis (PCA) on the IR spectra (Fig. S1) showed no clear class separation. These observations indicate that no major chemical changes are detectable over the ATR sampling depth.

To further investigate if we have chemical changes in the outermost fiber surface due to heat treatment, we analyzed using ToF-SIMS, which probes approximately the outermost 1–3 nm of the fiber surface [14]. Owing to its high surface sensitivity and mass resolution, ToF-SIMS is well suited for characterizing heterogeneous lignocellulosic surfaces and provides chemically resolved information on lignin, polysaccharides, extractives, and inorganic species [15–17].

PCA showed systematic variation among the three sample classes, with separation attributed to thermal treatment (Fig. 1a). To assess this class separation more explicitly, we applied orthogonal partial least squares-discriminant analysis (OPLS-DA), a supervised multivariate method that separates predictive (class-correlated) and orthogonal (class-uncorrelated) variation [9]. The corresponding global OPLS-DA score plot confirmed clear discrimination among the reference, 100 °C, and 200 °C classes (Fig. 1b). Centroid arrows indicate the direction of class displacement from the reference centroid to the hot-pressed samples. Detailed model statistics for the global PCA and OPLS-DA models, together with all pairwise models, are provided in the SI (Fig. S2–S3).

3.2. ToF-SIMS analysis of industrially hot-pressed CTMP sheets

Having established measurable temperature-dependent differences in static hot-pressed sheets, the next step was to investigate the influence of temperature on industrial hot-pressed sheets, which are the primary focus of this study. Due to the higher surface roughness of the laboratory-prepared handsheets, reliable ToF-SIMS interpretation was primarily limited to ions below approximately *m/z* 250. The smoother industrially hot-pressed sheets provided improved spectral quality for higher-*m/z* ions (*m/z* 800), enabling a more comprehensive interpretation of species. Furthermore, the industrially prepared sheets allowed direct comparison of the heated front-side and the opposing back-side surfaces, enabling temperature-driven chemical redistribution to be

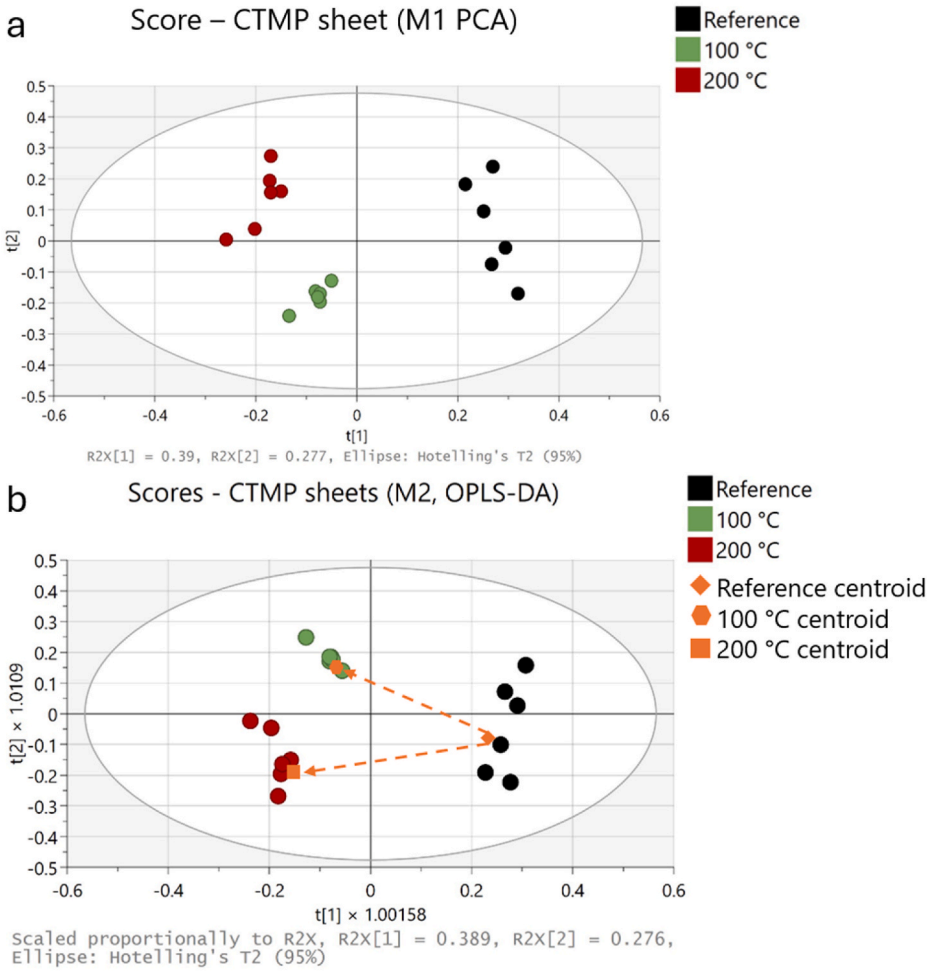

Fig. 1. Global PCA (a) and OPLS-DA (b) score plots of the laboratory static hot-pressed CTMP validation samples (untreated reference, 100 °C, and 200 °C), demonstrating temperature-dependent surface chemical discrimination prior to analysis of the industrially hot-pressed sheets.

distinguished from front/back-side-related variation.

To distinguish temperature-driven chemistry from front/back-related variation, we applied OPLS-DA to assess whether the four surfaces could be separated (Fig. 2). This test confirmed that the combined effect of temperature and sheet side is strong and predictive. To identify marker ions that reflect only temperature-driven molecular migration and not front/back-side related variation in chemistry, and thereby provide a robust, minimal mechanistic marker set for the hot-pressing-temperature effect, four pairwise OPLS-DA comparisons were performed.

To distinguish ions that respond specifically to temperature from those influenced by front/back-side related variation in chemistry, we used a shared and unique structures (SUS) plot [18–20]. In a SUS plot, the correlation-scaled loadings (*p(corr)*) for the same variables are taken from two OPLS-DA models built with partly overlapping class definitions and are cross-plotted against one another. In our case, *p*(corr) values from the 100 °C front/back-side model were placed on the x-axis, and *p*(corr) values from the front-side 100 vs 200 °C model were placed on the y-axis. The corresponding score plots showed clear class separation for the 100 °C front/back-side model (Fig. 3a) and the front-side 100 versus 200 °C model (Fig. 3b).

The SUS plot derived from these two OPLS-DA models is shown in Fig. 3c. The blue regions are defined as the areas that have absolute values $|p(corr)| \geq 0.6$ in the pairwise comparison in M6 (100 vs 200 °C front-side) and absolute values $|p(corr)| < 0.6$ in M5 (100 °C front-side vs back-side). Thus, the upper blue region contains ions enriched on the front-side at 200 °C, with high *p*(corr) in the temperature model (100 vs 200 °C, front-side) and low *p*(corr) in the side model (100 °C front vs back). In contrast, the lower blue region contains ions enriched on the front-side at 100 °C, with strong negative p(corr) in the temperature model and low p(corr) in the front/back-side model. Together, these two blue regions define the temperature-specific markers of interest in this study. In contrast, the green region highlights ions that are predominantly side specific at 100 °C (front/back-side) with negligible temperature dependence, and the orange region denotes ions that change coherently in both models (shared effects across contrasts). Variables near the origin have little or no discriminating power in either model. Based on this separation, the analysis henceforth focuses on the blue-marked regions in Fig. 3c.

The yellow stars within the blue regions denote selected marker ions previously identified in the literature [16,21]. Table 1 lists the corresponding *m/z* values and tentative species assignments for these starred ions. The full set of marker ions, assignments, and literature references is summarized in SI Table S1. To assess the relative temperature dependence of the identified ions, we analyzed TIC-normalized ToF-SIMS spectra (Fig. 4). The front/back-side controls at 100 °C and 200 °C (Fig. 4b–d) show no systematic front/back-side differences, supporting a temperature-driven effect rather than intrinsic front/back asymmetry. We therefore focus on the most significant differences in the identified ions between 100 °C and 200 °C.

Fig. 4a shows that, at 100 °C, the hot-pressed front-side is enriched in lignin- and carbohydrate-related ions (*m/z* 63, 87, 109), sterol ions (oxo-sitosterol $C_{29}H_{47}O^+$ at *m/z* 411; sitosterol $C_{29}H_{51}O^+$ at *m/z* 415) [21,22] and fatty acid salt adducts (e.g., lignocerate and pentadecanoate, with

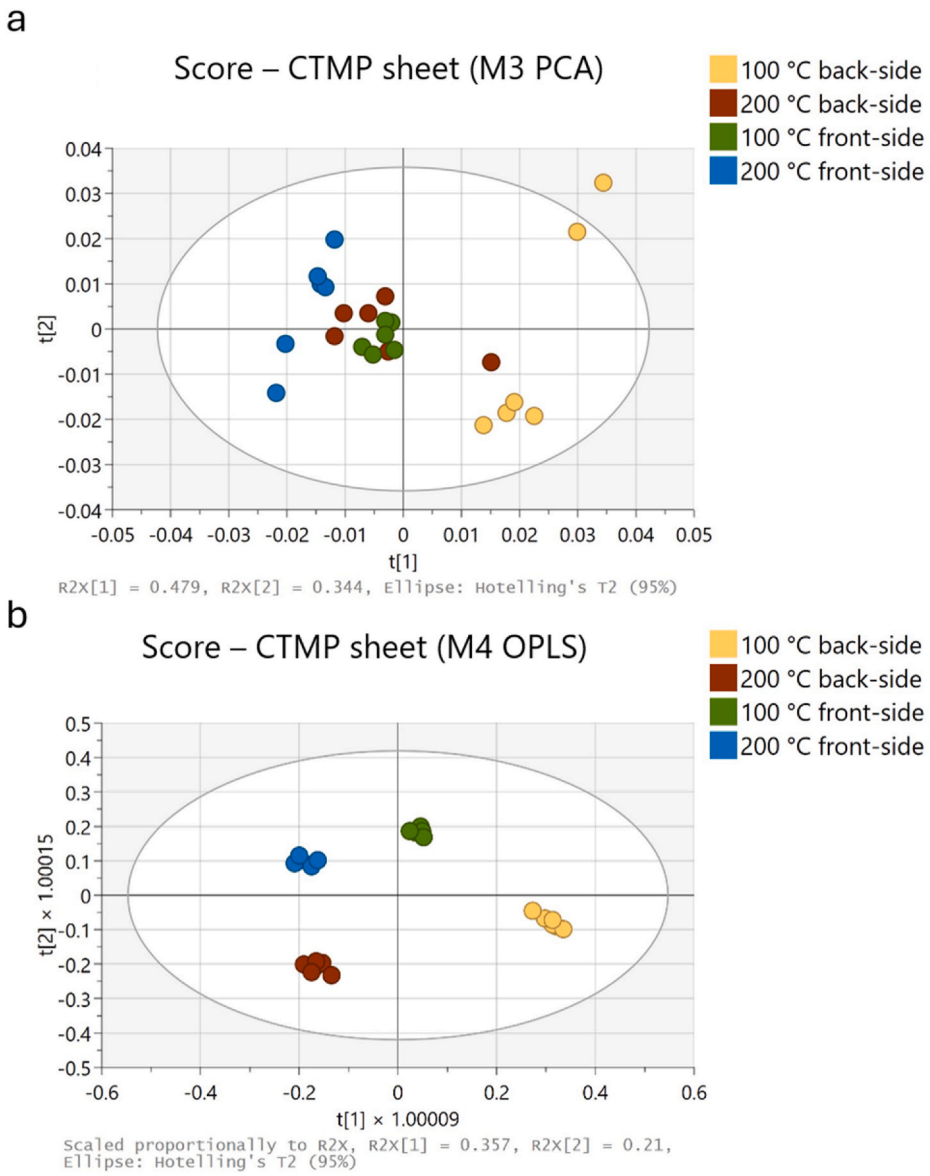

Fig. 2. PCA (a) and OPLS-DA (b) score plots of the CTMP temperature treated sheets.

m/z 413 and 523, respectively). These species are consistent with residual wood extractives known to persist in pulp fiber matrices [21] and are influenced by thermal behavior [23]. As seen in Fig. 4a and c, the differences in ion count for the small fragments are less abundant than for the larger fragments. Fig. 4c shows that, on the front-side at 200 °C, the surface is enriched in lignin-related aromatic ions ($C_6H_8O_3^+$ at *m/z* 128; $C_9H_9O_3^+$ at *m/z* 165), as well as long-chain fatty acid-derived fragments and metal-carboxylate adducts, including Ca-myristate and Ca-pentadecanoate (*m/z* 268, 296) [21,24] and C_{24}–C_{25} fragments (*m/z* 355, 369, 383). The precise origin of the observed Ca-containing adducts cannot be determined from the present data, but they could potentially indicate exposure to calcium-containing water or process streams during pulp washing or sheet preparation [17,25,26].

Notably, at 200 °C, the front-side shows clear enrichment in lignin-derived fragments and long-chain fatty acid salts; by contrast, at 100 °C, the front-side is instead characterized by relatively higher abundances of sterols and medium-chain fatty acids. Enrichment at the surface likely reflects thermal softening and enhanced mobility of lignin-derived fragments and extractives at higher temperature, which together promote migration to the surface and thus surface enrichment of these compounds. However, for the front-side of the 100 °C hot-pressed sheet, the surface-exposed polysaccharides, sterols, and medium-chain fatty acids are more apparent.

The literature indicates that surface reorganization is temperature-dependent due to moisture-assisted softening of lignocellulosic polymers during hot-pressing [4,27,28]. Residual moisture then acts as a plasticizer for the amorphous lignin and hemicellulose phases, lowering their effective glass-transition temperatures and increasing polymer-segment mobility under elevated temperature and pressure. This enhanced mobility can facilitate the redistribution of lignin-rich domains and hydrophobic extractives toward favorable surface regions.

Although localized degradation reactions cannot be entirely excluded, the temperatures employed in this study and the residence time under the heated nip (<1 s) limit the extent of thermal degradation. It is likely that the observed surface chemical differences can be interpreted primarily as the result of temperature-driven reorganization of existing chemical components [23,29].

In addition to improved smoothness, such extractive accumulation may be associated with altered surface properties [30]. In this work, temperature-driven surface changes are resolved using a chemometrics guided ToF-SIMS and SUS plot workflow, and the resulting marker set provides a robust basis for identifying mobile compounds.

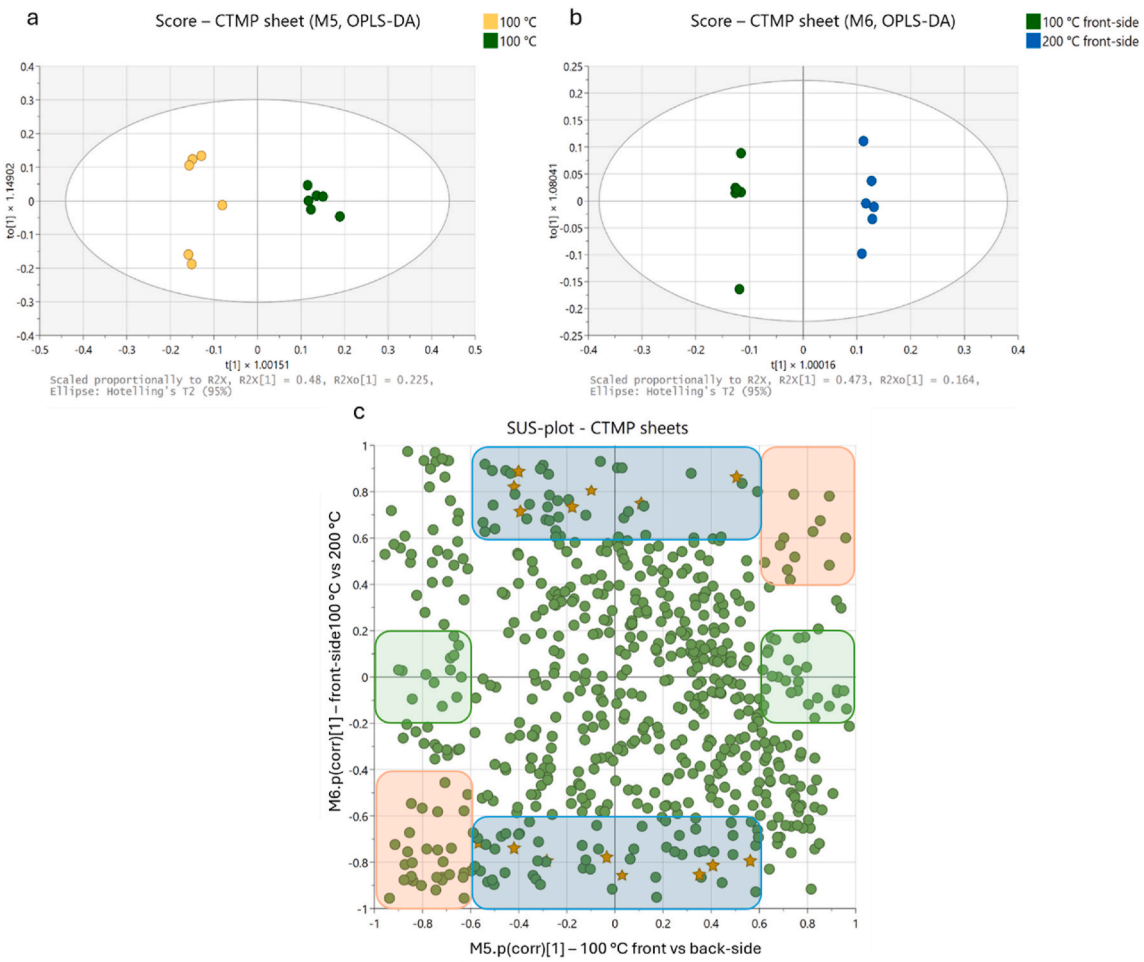

Fig. 3. OPLS-DA score plots for hot-pressed CTMP sheet showing (a) front-side 100 versus 200 °C and (b) front/back-side samples at 100 °C, and (c) the SUS plot comparing these two models. Yellow stars mark the selected temperature-responsive ions. Blue boxes indicate temperature-specific ions, orange boxes show ions shared by both models, and green boxes denote ions that are mainly side-specific at 100 °C.

Table 1
Temperature-enriched marker ions with tentative assignments.

m/z	Assignment	Temperature-Driven ions
63	$C_5H_3^+$	100 °C
87	$C_4H_7O_2^+$	100 °C
109	$C_6H_5O_2^+$	100 °C
411	$C_{29}H_{47}O^+$	100 °C
413	$C_{24}H_{48}O_2Na^+$	100 °C
415	$C_{29}H_{51}O^+$	100 °C
523	$C_{30}H_{59}O_4Ca^+$	100 °C
128	$C_6H_8O_3^+$	200 °C
165	$C_9H_9O_3^+$	200 °C
268	$C_{14}H_{28}O_2Ca^+$	200 °C
296	$C_{16}H_{32}O_2Ca^+$	200 °C
355	$C_{24}H_{51}O^+$	200 °C
369	$C_{24}H_{49}O_2^+$	200 °C
383	$C_{25}H_{51}O_2^+$	200 °C

4. Conclusions

Laboratory-prepared, statically hot-pressed CTMP handsheets showed that hot pressing induces chemical changes at the nanometer scale relative to untreated CTMP, whereas studies of industrially hot-pressed CTMP sheets revealed temperature-dependent surface reorganization using ToF-SIMS and chemometric analysis. While global multivariate analysis of industrially hot-pressed sheets captured contributions from both temperature and sheet side, the SUS-based workflow isolated a robust set of temperature-responsive marker ions independent of front/back-side asymmetry. The front side hot-pressed at 100 °C was relatively enriched in small carbohydrate- and lignin-related fragments, sterols, and medium-chain fatty acid salts, whereas the surface at 200 °C showed increased abundance of lignin-derived aromatic ions and long-chain fatty acid-related species. These findings support a temperature-driven redistribution mechanism involving enhanced mobility of lignin-related components and extractives at higher temperatures. The proposed workflow therefore provides a practical and chemically interpretable strategy for monitoring process-induced surface reorganization in lignocellulosic sheet materials.

Declaration of generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this work, the authors used Microsoft Copilot to improve the phrasing and clarity of this manuscript. All scientific content, interpretation, and final wording were reviewed and approved by the authors, who take full responsibility for the published text.

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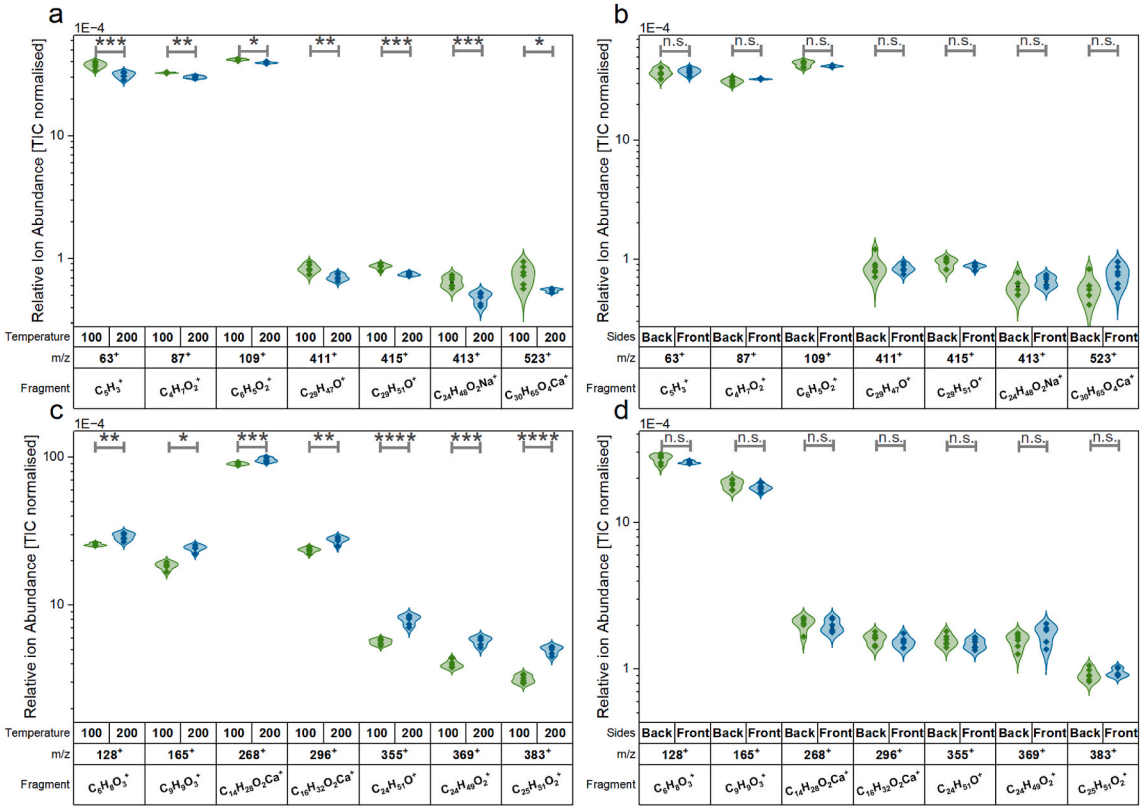

Fig. 4. Temperature-dependent behavior of selected marker ions on hot-pressed CTMP surfaces; a) TIC-normalized ion abundances on the front side at 100 and 200 °C for ions enriched at 100 °C; b) Front/back-side comparison at 100 °C for the same ions (side-control); c) TIC-normalized ion abundances on the front-side at 100 and 200 °C for ions enriched at 200 °C; d) Front/back-side comparison at 200 °C for the same ions (side-control); Welch's *t*-tests; *, $p < 0.05$; **, $p < 0.01$; ***, $p < 0.001$; ****, $p < 0.0001$; n. s., not significant.

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CRediT authorship contribution statement

Nivedhitha Venkatraman: Data curation, Formal analysis, Investigation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing. **Jutima Leksuntrakorn:** Data curation. **Anders Brolin:** Conceptualization, Supervision, Writing – review & editing. **Per Malmberg:** Conceptualization, Formal analysis, Methodology, Software, Supervision, Writing – review & editing. **Anette Larsson:** Conceptualization, Funding acquisition, Investigation, Project administration, Resources, Supervision, Validation, Visualization, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.polymertesting.2026.109301.

Data availability

Data will be made available on request.

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