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Review

Exploring Textile Fibre Characterisation: A Review of Vibrational Spectroscopy and Chemometrics

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Abstract

The identification/classification of textile fibres is essential in manufacturing, forensic science, cultural heritage preservation, and recycling. Conventional methods, including solubility tests, optical microscopy, and chromatographic techniques, are often destructive, labour-intensive, and limited in scope. Vibrational spectroscopy, particularly near-infrared (NIR), Fourier-transform infrared (FTIR), and Raman spectroscopy, has emerged as a rapid, non-destructive, and accurate alternative for fibre analysis. However, multi-composition textiles, dyes, finishing agents, and ageing effects frequently cause overlapping spectral features, hampering direct interpretation. This review examines the combined use of vibrational spectroscopy and chemometrics for textile fibre discrimination. It critically evaluates the performance of different spectroscopic techniques in classifying natural, synthetic, and blended fibres. The role of multivariate analysis methods, such as PCA, PLS, LDA, SIMCA, and machine learning algorithms, in improving spectral interpretation and classification accuracy is highlighted. Key factors affecting model robustness, including spectral pre-processing, sample heterogeneity, moisture, and colour, are also discussed. The integration of spectroscopy with chemometrics provides a robust, scalable, and sustainable solution for fibre identification, supporting quality control, fraud detection, and circular economy initiatives. This approach demonstrates significant potential for both research and industrial applications.

Keywords: mid-infrared; near-infrared; Raman; machine learning; multivariate data analysis; textiles; industry; recycling

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1. Introduction

The earliest approaches regarding textile fibre differentiation employed optical microscopy as the most common fibre types (cotton and linen) were straightforward to identify [1,2]. However, with the increasing number and diversity of synthetic fibres, microscopic differentiation has become more challenging [3]. Fibres were also subjected to a series of solubility and/or flame tests for identification. Lately, other techniques have also been employed or investigated, such as chromatographic methods coupled with mass spectrometry [4,5], differential scanning calorimetry (DSC), and DNA analysis [6]; however, all these methods are time-consuming, some require large sample quantities, and they are inherently destructive. In this context, researchers began to investigate the applicability of spectroscopic techniques for textile fibre discrimination [7,8]. Spectroscopy offers the

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advantage of textile analysis without sampling, particularly with the use of portable instruments that enable on-site measurements, thereby increasing the practicality of these techniques [9,10].

Vibrational spectroscopy, namely near-infrared (NIR), mid-infrared (MIR), Fourier-transform infrared (FTIR), and Raman spectroscopy, have proven to be rapid, cost-effective, non-destructive, and accurate analytical tools across multiple fields, including the food industry for fraud detection [11], freshness assessment [12], and nutritional composition prediction [13]; the feed industry [14]; medicine [15,16]; pharmaceutical analysis [17]; the fuel industry [18]; soil property prediction [19]; forensic science [20]; and microbiology [21]. The application of rapid and non-destructive techniques in textile analysis is crucial in several contexts. In the evaluation of historical textiles, preserving the integrity of cultural heritage artefacts is essential for continued study and conservation [10]. In forensic science, maintaining sample integrity while ensuring accurate fibre discrimination is important [22,23]. These techniques are also valuable upstream in the textile production process. Vibrational spectroscopy has been used to assess pulp quality prior to fibre production; for instance, Ren and Yuan [24] demonstrated that combining NIR spectroscopy with chemometrics enabled effective assessment of the quality of natural cellulose pulps intended for viscose rayon manufacturing. Textile recycling is another critical area, since the textile and fashion industry is among the most resource-intensive and polluting sectors due to its high consumption of water, energy, and chemicals, which significantly impact the environment [25]. The rise of fast fashion, characterised by low-cost, short-lifespan textiles, has further exacerbated this environmental burden. Riba and Cantero [25] emphasised that "to minimize the environmental footprint of the textile and fashion industry [. . .] textiles should be part of a circular economy, thus extending the life of textiles and clothes, while retaining textile fibres within a closed circuit." Effective recycling and reuse of textiles, however, depend on accurate fibre discrimination, which is also essential for fraud and counterfeit detection [26]. In this context, there is a pressing need for reliable methods to confirm textile composition. Although the textile industry employs various certifications to ensure product quality, sustainability, and social responsibility, these standards address specific aspects rather than providing comprehensive fibre composition verification. OEKO-TEX Standard 100 certifies that textiles are free from harmful substances but does not verify fibre content [27]. GOTS (Global Organic Textile Standard) [28] requires that products contain at least 70% certified organic natural fibres and covers processing, manufacturing, and labelling, but it focuses on organic origin rather than complete fibre-type identification (Global Standard gGmbH, 2024). Similarly, GRS (Global Recycled Standard) and RCS (Recycled Claim Standard) [29,30] verify the percentage of recycled content, and OCS (Organic Content Standard) tracks organic material from farm to final product, but none of these certifications independently confirm the accuracy of fibre-type composition claims on product labels (Textile Exchange, 2024). While standardised laboratory methods exist for quantitative fibre analysis, such as ISO 1833 for chemical dissolution methods and AATCC 20A for fibre identification, these are testing protocols rather than product certifications. Consequently, a gap remains in the certification landscape: no widely adopted certification specifically verifies that the fibre composition stated on textile labels accurately reflects the actual fibre content. This gap underscores the need for rapid, reliable, and non-destructive analytical methods capable of confirming textile composition, which is the central focus of this review. In addition to voluntary certification schemes, fibre composition labelling is subject to legal requirements in the European Union. Regulation (EU) No 1007/2011 of 27 September 2011 establishes harmonised textile fibre names and rules for the labelling and marking of fibre composition for textile products sold on the EU market, thereby requiring that the fibre composition declared on product labels is accurate and uses standardised fibre naming.

Spectroscopic techniques offer greener, sustainable and non-destructive ways to assess the fibre molecular structure and chemical composition [31], but they involve analysing many spectra, and manual examination of each spectrum is time-consuming and inefficient for fibre discrimination. Furthermore, spectra from different samples can appear highly similar, particularly when analysing complex matrices as those possessing dyes [32] and/or other chemical treatments [3,33]. To overcome these challenges, combining spectroscopic techniques with chemometric methods has emerged as a robust solution, mitigating issues related to peak overlap and spectral similarity.

This review aims to summarise the current state of the art regarding the application of spectroscopy and chemometrics for textile fibre identification.

2. Natural and Man-Made Fibre Classification

Figure 1 illustrates the classification of the main natural and man-made fibres employed in the textile industry. Textile fibres are commonly classified as natural (plant- and animal-derived) or man-made. Man-made fibres may be further divided into regenerated fibres (produced by chemical processing of natural polymers such as cellulose, e.g., viscose/lyocell) and synthetic fibres (produced by chemical synthesis, e.g., polyester, polyamide, acrylic). Inorganic/mineral fibres (e.g., glass or basalt) are typically processed and are mainly used in technical textiles and composites; they are therefore discussed here as a separate technical category rather than as “ready-to-use” natural fibres. Natural fibres refer to those occurring naturally and obtained from plants or animals. In this review, “mineral fibres” refers to inorganic fibres historically or technically used in textiles. Historically, asbestos was used in protective textiles due to its heat resistance, but it is now restricted/banned in many jurisdictions due to well-established health hazards. In modern applications, inorganic fibres such as glass and basalt are more commonly found in technical textiles and composite reinforcements, and metallic fibres may be used in niche functional fabrics (e.g., antistatic or shielding applications). Synthetic fibres, in contrast, are man-made fibres produced by chemical synthesis (typically from petrochemical feedstocks) [34–36]. Synthetic fibres currently dominate global production. In 2022, synthetic fibres accounted for 87.6 million metric tons, whereas natural fibres such as cotton and wool represented 25.2 million metric tons. Polyester is the most widely used textile fibre, representing 54% of global fibre consumption, while all synthetic fibres combined represent 64% of the total [37]. Comfort is influenced by multiple factors, including moisture management (moisture regain), air permeability, thermal conductivity, fibre morphology, yarn/fabric construction, and finishing treatments. While some natural fibres are often perceived as comfortable due to breathability and moisture absorption, this is not a universal rule; regenerated cellulosic fibres (e.g., viscose) can also exhibit favourable comfort-related properties, and synthetic fibres can be engineered (e.g., by cross-section design or finishing) to improve breathability and moisture transport [38]. These considerations highlight the need to improve synthetic fibres or develop new sustainable sources of textile fibres, such as agricultural by-products. A previous study employed FTIR spectroscopy to analyse fibres derived from rice husks and pineapple crowns, demonstrating that these lignocellulosic fibres exhibit properties comparable to commercial fibres, indicating their potential application in the textile industry [39]. Indeed, pineapple [40], banana [41], and nettle [42,43] fibres are applied to fabrics and can be characterised by FTIR. They are also used as alternative materials for building construction and employed for reinforcement in composite materials [44].

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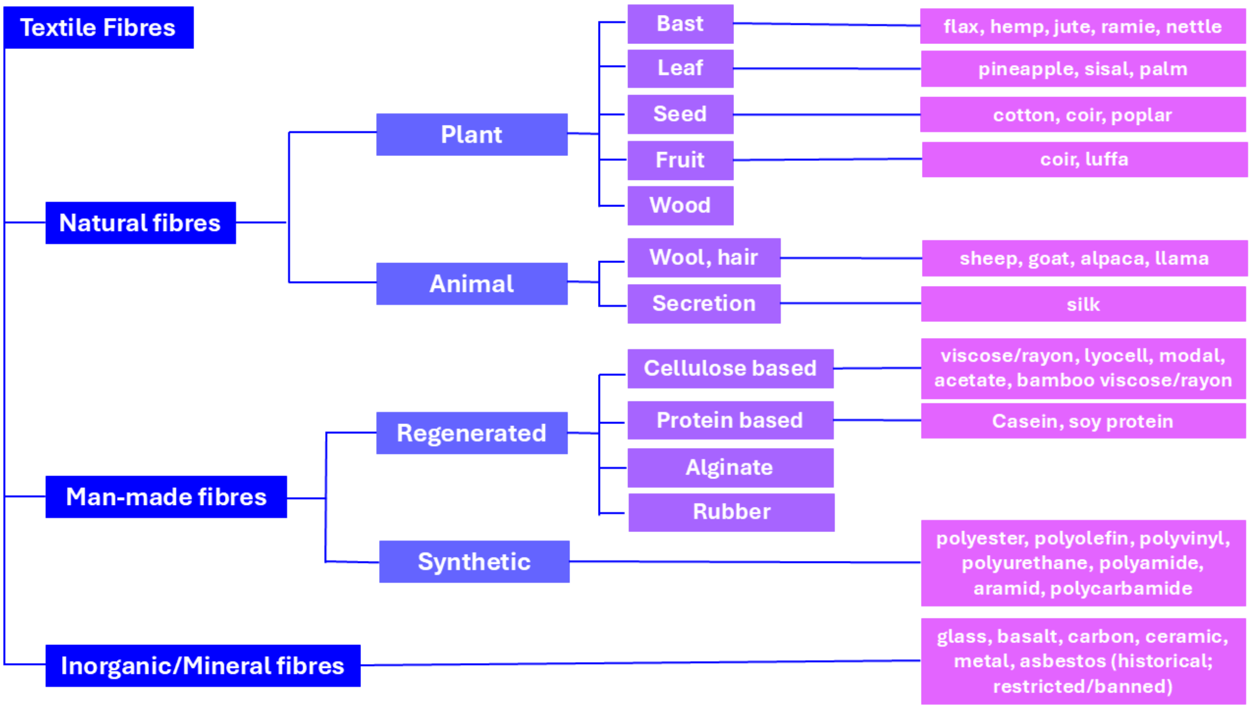

Figure 1. Classification of textile fibres into natural, man-made (regenerated and synthetic), and inorganic/mineral (technical applications) categories. Note: most commercial bamboo textile fibres are regenerated cellulosic (bamboo viscose/rayon); mechanically extracted bamboo bast fibre is classified as natural.

3. Vibrational Spectroscopy

Different polymers can be distinguished using vibrational spectroscopy because different functional groups exhibit distinct vibrational responses when excited by electromagnetic radiation. The resulting spectra display absorption bands corresponding to specific chemical groups, which in turn are associated with specific molecular structures. The main bands include O–H (absorbed water, serine), N–H (peptides, proteins), C–H (methyl and methylene groups in peptides, alanine, serine, bending in cellulose), and C=O (carboxyl and acetyl groups in hemicelluloses) [10,45,46].

This review focuses on three vibrational spectroscopy techniques, NIR, FTIR, and Raman, and summarises the current state of the art regarding their application in textile fibre analysis.

3.1. Textile Fibre Analysis by Vibrational Spectroscopy

Although fibres from similar sources often have comparable characteristics, making their differentiation challenging, vibrational spectroscopy has proven effective in distinguishing fibres with similar chemical structures. Several studies have demonstrated its applicability across diverse scenarios. For instance, natural fibres such as llama fleece [47], alpaca fibres [48], and cashmere from different animals [33] have been successfully discriminated, as have various cellulosic materials present in historical fabrics [49] and plant-based fibres like flax [50] or regenerated from plant cellulose (bamboo viscose/rayon). Accordingly, in textile contexts, “bamboo fibre” often refers to regenerated cellulosic fibre produced from bamboo-derived cellulose rather than mechanically extracted natural bamboo bast fibres. Spectroscopy has also been employed to differentiate fibres originating from different parts of the same plant, reflecting distinct maturation stages, such as cotton seed and lint [51]. Furthermore, it has enabled distinction between fibres of the same origin in different processing states; for example, natural bamboo fibres and bamboo pulp fibres were differentiated using NIR spectroscopy [52]. Ageing effects can also be assessed, as NIR and FTIR spectroscopies have been shown to detect chemical changes over time, allowing for the estimation of fabric age [3,53]. In addition to natural fibres, vibrational spectroscopy has been applied to discriminate between synthetic and natural fibres in various blends. FTIR spectroscopy has successfully distinguished wool, polyester, polyacrylonitrile, and nylon in mixed samples [54,55], while NIR spectroscopy has been used to classify a wide range of fibres and blends, including polyester, cotton, wool, silk, viscose, nylon, acrylic, and combinations such as polyester/cotton, polyester/wool, polyester/nylon, polyester/viscose, nylon/spandex, and silk/cotton [56]. Synthetic fibres can also be differentiated among themselves using NIR and FTIR techniques [31,57–59]. For less common fibres and technical textiles, IR spectroscopy also supports structural understanding and identification of materials such as aramids, UHMWPE, PEEK, polyimides, and PPS; PAN can be considered a common precursor fibre (e.g., for carbon fibre production) rather than a typical high-performance apparel fibre [60]. Some authors have suggested pre-treating cotton fabrics with aqueous sodium hydroxide to reduce variability related to mercerization (a process primarily applied to cotton to modify cellulose crystallinity and related properties), which can influence spectral features [45,61]. However, since vibrational spectroscopy is primarily valued for being non-destructive, simple, rapid, and accurate [26], such pre-treatment is rarely adopted in scientific studies. Recent advances in hyperspectral imaging, which combines spectroscopy with spatial resolution, enable pixel-by-pixel fibre identification across fabric surfaces. This approach is particularly valuable for detecting localised contamination, identifying foreign fibres, and assessing the homogeneity of fibre distribution in blended textiles, providing detailed compositional maps that conventional single-point measurements cannot achieve.

3.2. Complementarity of Vibrational Spectroscopy Techniques

Table 1 provides a comparative overview of the applicability of NIR, FTIR, and Raman spectroscopy in textile fibre analysis. The NIR region, located between the visible and mid-infrared ranges (13,000–4000 cm^{-1}; 2500–780 nm), results from the absorption of photons that excite complex molecular vibrations. This technique has been widely applied to predict fibre quality for textile applications. Canaza-Cayo et al. [48] demonstrated that NIR spectra in the 2500–1100 nm range correlate with key quality traits of alpaca fibres, such as mean fibre diameter and spinning fineness. NIR is also considered the most suitable technique for analysing historical fabrics, as it is less invasive compared to FTIR combined with attenuated total reflectance (ATR) or Raman spectroscopy. In ATR measurements, samples must be pressed against the crystal, which can be damaging to heritage textiles [10].

Table 1. Comparative analysis of NIR, FTIR, and Raman spectroscopy techniques.

Characteristic	**NIR**	**FTIR**	**Raman**
Principle	Measures absorption of near-infrared radiation; sensitive to overtones and combination bands.	Measures absorption of infrared radiation by polar chemical bonds.	Measures inelastic scattering of light due to molecular vibrations.
Sensitivity to functional groups	Detects overtones and combination bands of molecular vibrations (O-H, N-H, C-H overtones and combinations).	High for polar groups (O-H, C≡O, C=O, C–O, N-H).	High for covalent bonds and crystalline structures.

Table 1. *Cont.*

Characteristic	NIR	FTIR	Raman
Water interference	High; water absorption can interfere with measurements.	High; water strongly absorbs in the infrared region.	Low; minimal interference from water.
Dye/colour interference	Some interference from dyes; suitable for analysing dyed textiles.	Only dyes absorbing in the infrared region can interfere with measurements.	Only fluorescence from dyes can interfere on dyes differentiation, but using longer excitation wavelengths (e.g., 1064 nm) can mitigate this.
Best suited for	Rapid, non-destructive identification of fibre types and assessing overall chemical composition.	Identifying chemical composition of fibres and functional groups.	Analysing molecular structures and detecting specific dye-fibre interactions; identifying dyes (natural and synthetic)
Penetration depth	Deeper; can penetrate through thin fabrics.	Shallow; typically, a few µm.	Very shallow; surface-sensitive with penetration depths in the nm to µm range.
Ease of use	Minimal sample preparation; suitable for on-site and rapid assessments.	Minimal sample preparation.	The use of small samples requires more careful handling. Sensitive to fluorescence; requires careful selection of laser wavelength.
Method limitations	Strongly dependent on calibration models. Sensitive to physical sample variation. Low sensitivity to minor components.	Requires good contact between sample and ATR crystal. Functional groups often produce broad absorptions, limiting chemical specificity in complex mixtures.	Weak scattering efficiency. Sample heating and photodegradation. Limited applicability to highly absorbing materials.
Costs	Cheapest.	Moderate.	Most expensive.

FTIR spectroscopy, covering the 4000–600 cm^{-1} region, detects two main types of vibrations: stretching vibrations along chemical bonds (e.g., C–O and C–OH) and bending vibrations involving changes in bond angles [62]. FTIR-ATR has been extensively used for fibre identification, including cashmere [63], cotton [64], bamboo and flax [50], modal, viscose, linen, and dyed poplin-cotton [49], as well as a wide range of natural and synthetic fibres such as wool, silk, jute, sisal, cellulose acetate, lyocell, fibreglass, polyester, polyamide, polyacrylic, elastane, polyethylene, and polypropylene [59]. The main functional groups and main diagnostic signals for the most common fibre types are reported in Table 2 [59]. FTIR has also been applied to blended fabrics [65], including polyester/cotton [31,57], historical textiles and leather [66,67], wool/silk [68], cotton/elastane, polyester/elastane, cotton/polyester [53], and even blends of up to four fibres (wool, polyester, polyacrylonitrile, and nylon) [54]. Additionally, FTIR has been used to discriminate fibres at different maturation stages. Liu et al. [51] observed spectral differences between mature and immature cotton seeds, although sample homogeneity was noted as a critical factor.

Table 2. Main vibrations and functional groups of the main fibre types.

Fibre Type	Key Functional Groups	Main Bands (cm^{-1})	Main Diagnostic Signals (cm^{-1})
Cotton *	–OH, C–O, C–O–C	3330–3500 (O–H), 2900 (C–H), 1640 (H_2O), 1425 (CH_2), 1160 (C–O–C), 1050 (C–O), 895 (β-glycosidic)	1160, 1050, 895
Linen *	–OH, C–O, C–O–C	Same as cotton, with sharper 1425 and 895 bands	1425, 895
Viscose/Rayon *	–OH, C–O, C–O–C	Broader O-H band; weaker 1425/895; 2900 (C–H), 1160 (C–O–C), 1050 (C–O)	Broader 3330–3500, weak 895
Wool	Amide I–III, –NH, –C=O, –C–S–	3300 (N–H), 1650 (amide I), 1540 (amide II), 1230 (amide III), 700–600 (C–S)	1650, 1540, 600–700
Silk	Amide I–III, –NH, –C=O	3300 (N–H), 1620–1640 (amide I), 1515 (amide II)	1620–1640, 1515
Polyester (PET)	Aromatic C=C, ester C=O, C–O	1715–1730 (C=O), 1240–1260 (C–O), 1100 (C–O), 1600/1500 (aromatic), 720–870 (C–H bend)	1715–1730, 1240–1260, 1600
Polyamide (Nylon)	Amide I–III, –NH, C–N	3300 (N–H), 1650 (amide I), 1530 (amide II), 1290 (amide III), 936–1030 (C–N)	3300, 1650, 1530
Polypropylene (PP)	CH_3, C–H	2950/2870 (CH_3 stretch), 1455/1375 (CH_3 bend), 1167/997/841 (tacticity)	1455, 1375, 841
Polyethylene (PE)	CH_2, C–H	2915/2849 (CH_2 stretch), 1470/1460 (CH_2 bend), 730/720 (rocking)	1470, 720
Acrylic (PAN)	C≡N, CH_2	2240–2250 (C≡N), 1450–1350, 2900 (C–H)	2240–2250
Elastane (Spandex)	Urethane C=O, N–H, C–O–C	1700–1730 (C=O), 3320–3400 (N–H), 1530 (N–H bend), 1220–1260 (C–O–C)	1700–1730, 3320–3400

* Cellulose-based fibres are sometimes hard to differentiate, often requiring additional techniques.

Raman spectroscopy has been particularly valuable for dye analysis in textiles. Bruni and De Luca [69] compared FTIR and Raman spectroscopy for dyed wool threads and found Raman to be more effective in detecting dye-related spectral features as the FTIR spectra were dominated by wool signals, making dye identification through visual inspection challenging. While FTIR can provide structural information on dyes [70], it generally lacks characteristic dye bands, whereas Raman spectroscopy can detect colour-related features depending on dye concentration and sample colour [71]. Studies have shown that Raman spectra are dominated by dye signals at high dye concentrations, while fibre signals prevail at lower concentrations [46]. Despite its advantages, Raman spectroscopy is affected by fluorescence, which can obscure the weaker Raman signal from the fibre itself. This limitation can be effectively mitigated by using an excitation wavelength of 1064 nm (near-infrared region) and low laser power. At this longer wavelength, the photon energy is insufficient to excite the electronic transitions in most dye molecules, meaning the dyes do not fluoresce. Because the dye fluorescence is not activated, the weak Raman scattering signal from the fibre is no longer hidden by the intense fluorescence background, enabling clearer spectral acquisition even for heavily dyed fabrics. Additionally, the lower photon energy reduces the risk of sample photodegradation during repeated scans, making this approach particularly suitable for the analysis of coloured textiles and historical fabrics where sample preservation is essential. This approach has been successfully applied to qualitatively assess deterioration in linen fibres [72,73]. Although some studies recommend combining Raman with complementary techniques such as optical microscopy, infrared microspectroscopy, UV-Vis spectroscopy, and visible microspectrophotometry [32,74], Raman remains the most widely cited method for dye analysis in textiles.

One of the key factors in selecting an appropriate spectroscopic technique is the sample size, as illustrated in Figure 2. When analysing very small samples, FTIR and Raman spectroscopy are often required. FTIR can be applied to samples as small as approximately 15 µm, depending on the instrument, while Raman spectroscopy enables the analysis of microsamples as small as 1 × 1 µm. However, when dealing with fibre blends, achieving a homogeneous mixture of entire fibres is challenging, making it difficult to accurately predict textile composition from a limited analysis area [54]. In such cases, NIR spectroscopy, which allows for a broader analysis area, becomes advantageous. Additionally, increasing the number of replicates across different regions of the textile is recommended to account for sample heterogeneity, particularly when the objective is fibre quantification. Several authors have emphasised the importance of multiple replicates to minimise variability and improve the reliability of results [7,54,65].

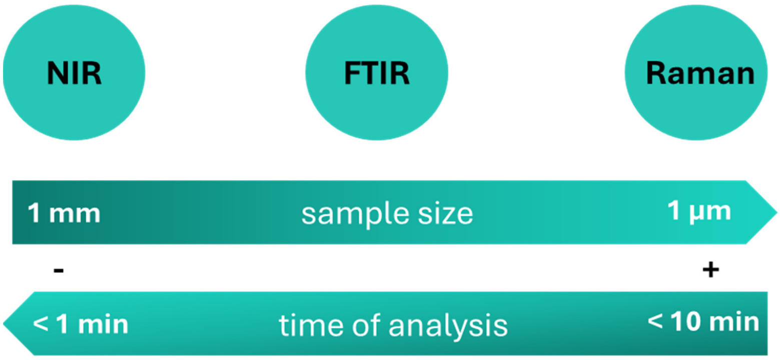

Figure 2. Time of analysis and sample size relations for the different vibrational spectroscopy techniques.

3.3. Limitations of Vibrational Spectroscopy in Textile Fibre Analysis

The limitations of each spectroscopic technique arise primarily from the influence of non-fibre components present in textiles, such as colourants, colour intensity, brightness, water content, and chemical agents [75]. These factors can lead to misclassification due to external treatments rather than intrinsic properties [74]. Coatings and finishing agents can also cause recognition errors [53]. Additionally, fabric thickness and ageing significantly affect NIR [53] and FTIR [67] analyses. Cura et al. [53] observed that NIR penetrated thin fabrics, resulting in failed fibre recognition, while ageing altered fibre chemistry, complicating identification. Although folding fabrics to increase thickness can mitigate this issue, FTIR studies have also reported misidentification in aged fibres [67]. Moisture content is another critical factor influencing spectra. While FTIR-ATR peak positions remain stable under varying humidity [67], NIR spectroscopy effectively measures residual moisture (0.05–50%) [75]. Furthermore, NIR has been adapted for cashmere identification in wet textiles by creating spectral libraries across moisture ranges and applying classification models tolerant to humidity variability [76]. This approach enables accurate, drying-free analysis under real-world conditions.

Overall, the main limitations of vibrational spectroscopy stem from fabric heterogeneity and external factors such as colour, moisture, and chemical treatments. Accurate fibre identification requires multiple spectra and replicates, which significantly increases analysis time. Moreover, basic statistical tools such as correlations and ANOVA are insufficient for distinguishing similar fibres (e.g., cashmere vs. wool) or accounting for overlapping spectra [63]. These challenges underscore the need for advanced multivariate and machine learning methods to achieve reliable fibre discrimination.

4. Vibrational Spectroscopy and Chemometrics for Fibre Identification

As discussed above, vibrational spectroscopy offers several advantages but also presents limitations in textile fibre analysis. One of the proposed solutions to overcome some of its challenges is the application of chemometrics. This approach is particularly relevant for fabrics containing multiple fibre types, where the complexity of the spectral data necessitates advanced computational methods, including machine learning techniques [55]. Multivariate analysis has demonstrated the ability to accurately identify fibres regardless of their origin, manufacturing residues, surface finishes, weave patterns, or dye content [77]. This section reviews the studies combining vibrational spectroscopy (FTIR, NIR, and Raman) with chemometric approaches for textile fibre discrimination. Table 3 summarises the main contributions in this area.

4.1. Chemometric Model Development and Validation: Workflow

The use of chemometrics for qualitative and/or quantitative fibre analysis in textiles follows the workflow illustrated in Figure 3. The first stage comprises model development, which includes two main steps [78,79]:

(i) Building the model using reference samples of single fibres and/or blends with known compositions;
(ii) Model validation with independent samples of known fibres or fabrics.

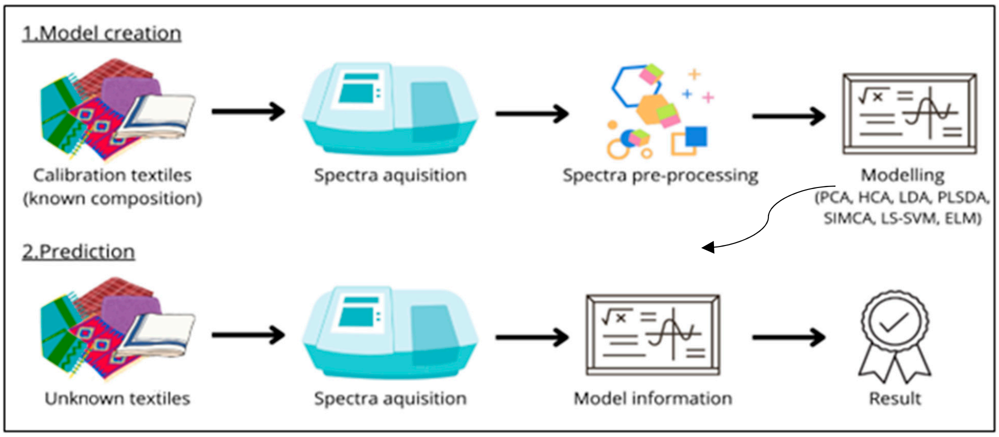

Figure 3. Workflow of the application of vibrational spectroscopy combined with chemometrics for textile samples analysis.

Once validated, the model can be applied to unknown sample prediction. The spectrum of the fabric under analysis is acquired and processed by the model, which identifies the fibre and/or composition based on its spectral characteristics.

4.1.1. Fabric or Fibre Selection

The process of model development (Figure 3) begins with the selection of fabrics or fibres. Several studies have employed single fibres or fabrics composed of only one fibre type [33,50]. Others have used fibre blends with known proportions to enable both identification and quantification of fibres in textiles [80,81]. Additionally, some authors have created spectral libraries from single-fibre fabrics and subsequently applied these models to identify fibres in blended textiles [68,82]. The choice between single fibres and blends depends primarily on the study's objectives. Table 3 also summarises the approaches adopted in different studies.

4.1.2. Spectral Acquisition Using Vibrational Spectroscopy

The subsequent step involves spectral acquisition. No clear trend was observed regarding the preference for FTIR or NIR; however, Raman spectroscopy is predominantly used when the study focuses on dyes. Both FTIR and NIR are widely applied for fibre identification and quantification in natural and synthetic fabrics, often in combination with Fourier transform (FT) techniques (see Table 3). For FTIR, the ATR crystal is typically cleaned with ethanol, and background measurements are obtained using air. In some cases, a standard such as polystyrene is used to verify instrument performance [82]. NIR spectra are generally collected in the 10,000–4000 cm^{-1} range, with the visible region excluded to avoid variability caused by pigmented fibres [47]. Raman spectroscopy commonly employs a neodymium: YAG laser with an excitation wavelength of 1064 nm, particularly in dye analysis [69,83], although other configurations are also reported [3]. Across all techniques, the number of replicates per sample typically ranges from three to five.

4.1.3. Spectral Pre-Processing

Prior to modelling, spectral data undergo pre-processing to reduce systematic noise and enhance the chemical information relevant to fibre identification. The first step often involves removing wavelength regions unrelated to the study objective, such as excluding the visible range when analysing pigmented fibres to avoid colour-related variability [47]. Derivative treatments are commonly applied to correct baseline shifts and improve spectral resolution [47,82,84]. Combined pre-processing algorithms are frequently employed. Bonifazi et al. [85] applied Standard Normal Variate (SNV) to correct baseline variations and scaling differences, followed by the Savitzky–Golay first derivative and mean centring. Sun et al. [73] implemented a sequence of steps including Multiplicative Scatter Correction (MSC), Savitzky–Golay derivatives (first and second order), and smoothing to eliminate baseline drifts, enhance small spectral differences, and reduce random noise. Their results indicated that the best pre-processing combination for cotton/polyester blends was second derivative plus Savitzky–Golay smoothing and MSC. Similarly, Chen and Men [86] demonstrated that applying the Variable Iterative Space Shrinkage Approach (VISSA) to optimise characteristic wavelengths significantly improved model performance.

4.1.4. Modelling

After pre-processing, spectra are used to develop predictive models. Various chemometric and machine learning techniques have been successfully applied, including Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), Soft Independent Modelling of Class Analogy (SIMCA), Partial Least Squares (PLS) regression, Convolutional Neural Networks (CNNs), Least Squares Support Vector Machines (LSSVMs), and Extreme Learning Machines (ELMs) (see Table 3). These methods support multiple objectives, such as fibre identification, origin determination [63], quality prediction [48,84], fibre quantification in blends [81,82], and classification of waste fibres [87]. It is noteworthy that all studies aiming to quantify fibres employed multivariate analysis. In contrast, studies without modelling typically focus on structural analysis, such as evaluating chemical changes in wool treated with azo dyes [70] or analysing silk fibroin structure [83].

Table 3. Vibrational spectroscopy (FTIR, NIR, and Raman) combined with chemometrics for textile fibre discrimination.

Studied Fibre (Total Sample Count = n) *	Fibre		Spectroscopic Technique	Multivariate Analysis [1] and Performance Score	Aim of the Study	Year	Ref.
	Single	Blend					
Natural Fibres							
Natural llama fleeces of 7 colours (white, black, grey, brown, light brown, coffee, and beige) (n = 169)	✓	---	NIR (700–2500 nm)	M-PLS regression; $R^2 = 0.67$; SECV = 1.965; SEV = 2.235 and RPD = 1.91	Predict mean fibre diameter	2021	[47]
Cotton, wool, and silk (n = 13). Unaged, naturally aged, artificially aged. Undyed, dyed with natural dyes, dyed with synthetic dyes	✓	---	NIR (1000–1700 nm) and Raman	PCA-LDA e SIMCA	Compare PCA-LDA and SIMCA	2022	[3]
Sticky cotton (n = 457)	✓	---	NIR (10,000–4000 cm^{-1})	SECV = 0.26; $R^2 = 0.96$	Analysis of the "stickiness" of the cotton prior fabric production	2005	[84]
Dyed wool threads (natural dyes) (n = n.d. [2])	✓	---	FTIR (4000–400 cm^{-1}, then 1800–950 cm^{-1}); FT-Raman (Nd:YAG laser provided sample excitation at 1064 nm; 3500–100 cm^{-1}, then 1750–450 cm^{-1})	n.a.	Identify dyes	2011	[69]
Alpaca fibre samples from mid-side of the animals (n = 291)	✓	---	NIR (400–2498 nm)	PCA	Predict alpaca fibre quality for textile applicability	2013	[48]
Sheep cashmere, cashmere, rabbit, and camel fibres (n = 376)	✓	---	NIR (10,000–4000 cm^{-1})	PCA-LDA e SIMCA	Identification of fibres	2019	[33]
Pure goat cashmere from different provinces, rabbit and camel hair, cashmere–rabbit hair blends, cashmere–acrylic–polyester blends, cashmere–acrylic–polyester–cotton blend, wool, natural silk, cotton (n = 463)	✓	✓	NIR (10,000–4000 cm^{-1})	Relief algorithm; new: data driven based class-modelling (DD-SIMCA)	Identification of cashmere in blends	2019	[80]
Wool and cashmere (n = 210)	---	✓	NIR (1000–2500 nm)	LSSVM $R^2 = 0.9821$, RMSE = 1.1263, and MAE = 0.6527	Quantitative determination of wool and cashmere mixed fibre	2024	[86]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	**Fibre**		**Spectroscopic Technique**	**Multivariate Analysis** [1] **and Performance Score**	**Aim of the Study**	**Year**	**Ref.**
	Single	**Blend**					
White and purple cashmere, domestic Xinjiang fine wool, and soil-type combed cotton wool (n = n.d.)	✓	✓	NIR (1400–2500 nm due to the colours)	PLS-DA and LDA	Non-destructive identification of cashmere and wool	2025	[88]
Wool and cotton (n = n.d.)	---	✓	NIR (2250–2400 nm)	SIMCA	Identification of contamination of natural fibre yarns with polymeric fibrils	1998	[89]
Foreign fibres in cotton layers (n = 100)	---	✓	NIR (780–2360 nm)	CNN and TCN	Identification of foreign fibres in cotton layers	2023	[90]
Wool and silk and blended fibres (n = 128)	✓	✓	ATR-FTIR (4000–650 cm^{-1})	n.a.	Identification of fibres in blended textiles	2006	[68]
Plant- and chemical-dyed cotton fabrics (n = 336)	✓	---	FTIR (4000–500 cm^{-1}) NIR (10,000–4000 cm^{-1})	PCA, SIMCA > 95%, PCR: R^2 = 0.9937, RMSEE = 0.1332, PLS: R^2 = 0.9978, RMSEE = 0.0779	Identification of plant-dyed and chemical-dyed textiles	2020	[91]
Bamboo and flax (n = 25)	✓	---	FT-NIR (12,000–4000 cm^{-1})	Ward's algorithm and HCA = 100%	Identification of natural bamboo fibres and flax fibres with NIR	2013	[50]
Seed and lint cottons (n = 402)	✓	---	FTIR (900–1200 cm^{-1})	Correlations to compare traditional method and FTIR, R^2 = 0.89	Discrimination of immature cottons from mature ones; determination of cotton maturity	2011	[51]
Cashmere (Chinese, Australian, Iranian), wool (Chinese, Australian), bison wool, qiviut from Muskox, vicuña and guard hairs (n = n.d.)	✓	---	FTIR (4000–600 cm^{-1})	correlations, ANOVA	Differentiation of animal fibres from different origins	2011	[63]
Wool, analysis of dyes changes during process (n = n.d.)	✓	---	FTIR (3080–940 cm^{-1})	n.a.	Evaluation of structural changes in wool fibre keratin treated with azo dyes	2000	[70]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	**Fibre**		**Spectroscopic Technique**	**Multivariate Analysis [1] and Performance Score**	**Aim of the Study**	**Year**	**Ref.**
	Single	**Blend**					
Natural cellulose pulp samples (n = 92), including 30 cotton pulps, 44 wood pulps, 16 cotton–wood mixed pulps and 2 bamboo pulps	✓	---	NIR (10,000–4000 cm^{-1})	PCA, PLS and SIMCA = 100%	Reactivity determination of natural cellulose pulp for viscose rayon by NIR. Natural cellulose (from cotton, wood and cotton-wood mixed pulps) reactivity for viscose rayon "reactivity of natural cellulose pulp is a key parameter in dissolving pulp in the viscose-fibre production process"	2015	[24]
Silk fibroin (n = n.d.)	✓	---	FT-Raman (3500–500 cm^{-1}; laser operating at 1064 nm); FTIR (1800–1100 cm^{-1})	n.a.	Analyse the structure of silk fibroin	2005	[83]
Linen/cotton blends (n = n.d.)	---	✓	FT-NIR (10,000–4000 cm^{-1})	PLS, PCs, R^2 = 0.994–0.998, RMSEC = 1.20–2.38, RMSECV = 1.54–4.73, RMSEP = 2.20–4.98	Predict the linen % in linen/cotton blends	2005	[81]
Bamboo, jute, flax, bamboo pulp fibres (n = n.d.)	✓	---	FTIR (4000–400 cm^{-1})	correlations	Identification of natural bamboo using FT-IR and 2D-IR correlation spectroscopy	2025	[45]
Pure cashmere textiles (n = 49), cashmere–wool blended textiles with wool contents ranging from 51.5 to 96.2% (*w*/*w*) (n= 51) and pure wool textiles (n = 20); samples (n = 120)	✓	✓	diffused reflectance NIR (portable NIR) (896–2115 nm)	SIMCA, SVM, and NRS	Identification and discrimination of pure cashmere and adulterated (wool) samples	2019	[76]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	Fibre		Spectroscopic Technique	Multivariate Analysis [1] and Performance Score	Aim of the Study	Year	Ref.
	Single	Blend					
Cashmere (n = 100), wool (n = 120), rabbit hair (n = 95) and camel hair (n = 80); samples (n = 395)	✓	---	NIR (4000–10,000 cm^{-1})	SVDD, KNNDD and GAUSS methods	Distinguishing cashmere from other animal fibres to avoid fraud	2019	[26]
Natural bamboo fibre, bamboo pulp fibres and ramie fibres (n = n.d.)	✓	---	NIR	first derivatives and database building	Discrimination of bamboo fibre and ramie fibre by NIR	2010	[52]
Natural dyes (anthraquinones, flavonoids, neoflavonoids, biflavonoids and phenazone derivatives (orcein)) in wool fibres and ancient textiles (n = n.d.)	✓	✓	FT-surface-enhanced Raman (4000–200 cm^{-1}) using for excitation the 1064 nm emission	n.a.	Identification of natural dyes in wool textiles and then in ancient textiles	2014	[73]
Silk, animal hair (wool, camel hair, yak hair), cotton, and bast (linen, ramie, hemp) (n = 13)	✓	---	Portable spectroradiometer: visible and near-infrared (VNIR) (350–1000 nm), SWIR1 (1000–1850 nm) and SWIR2 (1850–2500 nm).	PCA, MANOVA	To further explore the potential of discriminating the fibre types using portable spectroradiometer	2019	[9]
Waste cotton from different countries (n = 350)	✓	---	NIR (10,000–4000 cm^{-1})	SIMCA and PLS	Classification of waste cotton from different countries using NIR	2023	[87]
Wool and cashmere blends (0–100% each) (n = 22)	---	✓	NIR (handheld acousto-optic tuneable filter near-infrared (AOTF-NIR)) (1100–2300 nm)	MANOVA, Multilinear Regression Model and Prediction Performance, two multilinear regression (MLR), $R^2 = 0.997$, SEC = 2.668, and RMSEC = 2.836 (whole set)	Measuring of fibre contents of wool–cashmere blends	2017	[92]
Raw material of wool, cotton, and silk (n = n.d.)	---	✓	NIR	not known (only abstract available)	Discrimination of natural fibre variety and detection of foreign fibre	2008	[8]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	**Fibre**		**Spectroscopic Technique**	**Multivariate Analysis [1] and Performance Score**	**Aim of the Study**	**Year**	**Ref.**
	Single	**Blend**					
Wool (n = 20), white cashmere (n = 20), pigmented cashmere (n = 8), pigmented yak (n = 5), angora rabbit (n = 5)	✓	---	Non-pigmented samples were tested by using FTIR. All contaminated or oxidised samples were excluded from NIR analysis. NIR (10,000–3700 cm^{-1})	SIMCA, 1 method for each fibre, $R^2 = 0.95$	Identification of wool, cashmere, yak, and angora rabbit fibres and quantitative determination of wool and cashmere in blend by NIR	2013	[78]
Synthetic fibres							
Synthetic fibres (acrylic (n = 26), rayon (n = 12), nylon (n = 48), and polyester (n = 52) (n = 138)	---	✓	FTIR (4000–400 cm^{-1})	PCA and SIMCA	Qualitative analysis on 138 synthetic fibres (nylon, polyester, acrylic, and rayon) using ATR–FTIR	2022	[82]
PE (polyethylene); PPTA (para-amid); PP (polypropylene); PES (polyester); PA (polyamide); AC (acrylic) (n = 49)	✓	✓	Hyperspectral imaging technology (900 to 2500 nm)	PCA-LDA = 100%	Discrimination of the chemical content of fibres in different colours and structures	2017	[93]
(i) Textile-grade acrylic fibre: -Wet spun-monocomponent -Dry spun-monocomponent // bicomponent (ii) Special acrylic fibre (n = 100)	✓	---	Diffuse reflectance infrared Fourier transform (DRIFT) (4000–400 cm^{-1}) and SEM	n.a.	Characterisation of various acrylic fibres by FTIR	2003	[94]
Black and dark coloured fleece garments. Almost all made of 100% pes (n = 201)	✓	---	Microscopy (bright field, polarised light, fluorescence); Microspectrophotometry (MSP-visible range); FTIR and comparison microscopy	n.a.	Analysis of fleeces to further identification among other fibres	2016	[95]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	**Fibre**		**Spectroscopic Technique**	**Multivariate Analysis [1] and Performance Score**	**Aim of the Study**	**Year**	**Ref.**
	Single	**Blend**					
Dyed cotton fabrics modified by silver nanowires (AgNWs) (n = n.d.)	✓	---	Surface-enhanced Raman spectroscopy (SERS) (200–3200 cm^{-1})	n.a.	Analyse the potential of dispersive Raman spectroscopy and SERS phenomenon application in dyed cotton fabrics modified with silver nanowires	2019	[71]
Natural + synthetic fibres							
End-of-life textiles (n = 36)	✓	✓	SWIR (1000–2500 nm)	PLS-DA, $R^2 = 0.977$	(1) recognition of the fibre origin (plant-derived, animal-derived, artificial textiles such as synthetic and/or man-made cellulosic fibres) and, (2) discrimination of fabrics according to the material classes (silk, cotton, wool, viscose, linen, jute, polyester and blends)	2024	[85]
Wool, PES, polyacrylonitrile, and nylon blends (one, two, three or the four fibres) (n = 64)	---	✓	FT-NIR (4000–10,000 cm^{-1})	PLS; UVEPLS algorithm; RMSECV	Simultaneous determination of several fibres in blended textiles	2019	[54]
Mixtures of wool, polyester, polyacrylonitrile, and nylon (n = 64)	---	✓	FT-NIR (4000–10,000 cm^{-1})	PLS and ELM (extreme learning machine), RMSEC = 0.065, RMSEP = 0.05, and RPD = 5.64	Quantitative determination of fibre components	2019	[55]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	**Fibre**		**Spectroscopic Technique**	**Multivariate Analysis ^{1} and Performance Score**	**Aim of the Study**	**Year**	**Ref.**
	Single	**Blend**					
Cotton (CO), polyester (PES), viscose (CV), silk (TS), wool (WO), polyacrylonitrile (PAN) and acetate (CA) and all combinations of two factor blends (n = 28)	✓	✓	NIR (1450–1850 nm, range not influenced by moisture)	n.a.	Develop NIR as a method for quantitative and qualitative identification of textiles, moisture measurements, textile coatings and process control	2000	[75]
Cotton, PES, viscose, cotton/elastane, PES/elastane, cotton/PES (n = 253)	✓	✓	FTIR (400–4000 nm), optical microscopy	n.a.	Textile recognition and sorting for recycling at an automated line using NIR	2021	[54]
Acetate, cotton, polyester, rayon, silk and wool (n = 758)	✓	---	diffuse NIR (1000–2500 nm)	SIMCA	Identification of fibres	2015	[77]
Waste textiles: polyester, cotton, wool, silk, viscose, nylon, acrylic, polyester/cotton, polyester/wool, polyester/nylon, polyester/viscose, nylon/spandex and silk/cotton (n= 2764 to training and n = 526 to test)	✓	✓	NIR (901–2500 nm)	artificial intelligence, construction of models by CNN and Baidu deep learning platform PaddlePaddle > 95%	Identification of fibres in waste textiles for recycling	2022	[56]
Historical textiles and leather (cotton, hemp, viscose, silk, wool, leather, polyamide, acrylic, polyester) (n = 87)	---	✓	ER-FTIR (7500–375 cm^{-1})	n.a.	ER-FTIR as non-invasive substitute of microscopic examination and ATR-FTIR	2024	[66]
Cellulosic materials from traditional Japanese samurai armour (n = 8). Reference materials: non-woven hemp thread, Kozo and Manila hemp fibres, aged flax	✓	✓	ATR-FTIR (4000–600 cm^{-1}) and SEM	n.a.	To discuss the potential and limitations of ATR-FTIR spectroscopy for studying cellulosic fibres	2022	[67]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	Fibre		Spectroscopic Technique	Multivariate Analysis [1] and Performance Score	Aim of the Study	Year	Ref.
	Single	Blend					
Cellulosic and cotton fabrics: cotton (bleached voile and muslin, boiled poplin), modal, viscose, linen, and dyed poplin-cotton (n = n.d.)	✓	---	FTIR (4400–400 cm^{-1})	PCA, SIMCA	Discrimination of cellulosic fabrics by diffuse reflectance FTIR and chemometrics	1995	[49]
Cotton–polyester (0–100% cotton) (n = 214)	✓	✓	NIR (900–1700 cm^{-1})	LSSVM, PLS, SPA-LSSVM. LWA and RCA were also employed for effective wavelength selection. RMSEC = 0.77, RMSEP = 1.17	NIR spectroscopy to quantify the composition of cotton-polyester textiles.	2018	[57]
To create the model: pure PES slash, pure PES normal, pure wool, pure cotton, PES/nylon, PES/wool, PES/cotton slash, PES/cotton, nylon (n = 263)	✓	✓	NIR (780–2526 nm)	CNN	Qualitative classification of waste textiles using NIR and the convolutional network	2019	[58]
Cotton, polyester, linen, viscose, elastane, polyamide (n = 84)	---	✓	NIR (10,000–4000 cm-1) ATR-FTIR (4000–600 cm-1)	PCA, PLSDA e PLS All the prediction errors < 8%	Discrimination of cotton and polyester among textile fibres	2024	[31]
Wool, silk, cotton, linen, jute, sisal, viscose, cellulose acetate (acetate), Tencel™ (lyocell), fibreglass, polyester, polyamide, polyacrylic, elastane, polyethylene, and polypropylene (n = 61)	✓	---	r-FTIR (600–4000 cm^{-1}) ATR-FTIR (225–4000 cm^{-1})	PCA	Identification of fibres	2019	[59]
Cotton, silk, wool, linen, lyocell, viscose, PES, polyamide, polyacrylic, elastane and blends (n = 89)	✓	✓	ATR-FTIR (225–4000 cm^{-1})	PCA	Identification of fibres	2017	[65]
200 natural fibres (50 cotton, 50 linen, 50 wool and 50 silk samples) and 150 samples from artificial and synthetic fibres (50 viscose, 50 polyamide and 50 polyester samples (n = 350)	✓	---	ATR-FTIR (4000–400 cm^{-1})	PCA followed by CVA algorithm = 100%	Identification of fibres	2020	[25]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	**Fibre**		**Spectroscopic Technique**	**Multivariate Analysis** [1] **and Performance Score**	**Aim of the Study**	**Year**	**Ref.**
	Single	**Blend**					
Cotton, polyester (0–100% each) (n = 318)	---	✓	FT-NIR (3800–10,000 cm^{-1})	PLS, PCA, GA, RMSEC = 1.61–2.13, R^2 = 0.994–0.998, RMSECV = 2.07–2.54, RMSEP = 2.30–2.93	Quantitative analysis of cotton–polyester content in blend products	2006	[96]
Six types of fabrics made of cotton, linen, ramie, rayon, Cupra, and lyocell (n = 81)	✓	---	ATR-FTIR (1700–800 cm^{-1})	PCA, FDOD (Fisher's Discriminant analysis Orthogonal Decomposition)	Discrimination of fibres among natural fibres cotton, linen, ramie, and discrimination of fibres among synthetic fibres rayon, Cupra, lyocell	2021	[61]
Cotton (n = 28), wool (n = 15), terry wool (n = 30), synthetic fibre (n = 31) (n total = 104)	✓	---	FTIR (4000–450 cm^{-1})	PCA and multiple algorithms = 100%	Identification of fibres	2024	[23]
Textiles containing foreign fibre: Single jersey knit fabric (85% micro modal and 15% silk) contaminated with foreign fibre; Yarn contaminated with foreign fibre; Yarn with the same expected composition as foreign fibre contaminating yarn (n = 3)	---	✓	ATR-FTIR (400–4000 cm^{-1})	n.a.	Identification of a foreign polymer in textile matrix	2011	[97]
Cotton 100%, viscose 100%, acrylic 100%, polyamide 100%, polyester 100%, and blend of cotton–viscose 97%/3%. The fabrics were divided into training and prediction sets (60:60) for developing models and evaluating the classification abilities of the models (n = 120)	✓	✓	FT-NIR (10,000–4000 cm^{-1})	SIMCA, LSSVM, and ELM = 100%	Identification of fibres	2016	[98]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	Fibre		Spectroscopic Technique	Multivariate Analysis [1] and Performance Score	Aim of the Study	Year	Ref.
	Single	Blend					
Cotton and polyester blend fabrics (n = 194)	---	✓	FT-NIR (4000–12,493 cm^{-1})	MCUVE, SPA, PLS, and GA were performed comparatively to choose characteristic variables associated with cotton content distributions. $R^2 = 0.988$, RMSEP = 2.100	To measure cotton content in blend fabrics of cotton and polyester	2016	[99]
Cotton and viscose dyed fibres (n = n.d.)	✓	---	Raman (200–1800 cm^{-1})	n.a.	Discrimination between cotton and viscose fibres, dyed with several dye classes	2013	[46]
Blends of polyester and cotton dyed fibres (n = 16)	---	✓	Raman Spectroscopy (excitation sources: 514, 633, 785 nm) and Ultraviolet–Visible (UV-Vis); Microspectrophotometry (200–800 nm)	n.a.	Identification of dye mixtures in polyester and cotton fibres	2015	[100]
Cotton, flax, wool, silk and Tencel (40 each) (n = 200)	✓	---	Vis/NIR	PCA and LSSVM	Identification of fibres	2010	[101]
Acrylic, wool/cashmere, cotton, elastane, Kevlar, Nomex, PA6/PA66, pet, silk (n = 72)	✓	---	NIR (900–2606 nm)	PCA, SIMCA and Euclidian distances	Identification of fibres	2018	[102]
Wool, cashmere, terylene, polyamide, polyurethane, silk, flax. Linen, cotton, viscose, cotton–flax blending. Terylene–cotton blending, and wool–cashmere blending (n = 214)	✓	✓	NIR	SIMCA based on PCA	Identification of fibres	2010	[103]
100% cotton, PES, and cotton, 5 different coloured cottons, textiles of different fibres (acrylic, cotton, nylon, polyester, and silk) (n = n.d.)	✓	✓	Raman imaging (3000–200 cm^{-1})	PCA, MANOVA and MCR	Identification of textile fibres and dyes	2022	[74]

Table 3. *Cont.*

Studied Fibre (Total Sample Count = n) *	Fibre		Spectroscopic Technique	Multivariate Analysis [1] and Performance Score	Aim of the Study	Year	Ref.
	Single	Blend					
Waste fabrics of polyester, polyamide, acrylic, silk, and wool (n = 186)	✓	---	NIR (10,000–4000 cm^{-1})	SIMCA > 90%	Identification of fibres from waste fabrics	2018	[79]
Cotton, Tencel, wool, cashmere, polyethylene terephthalate (PET), polylactic acid (PLA), and polypropylene (PP) (n= 7)	✓	---	NIR (1100–2300 nm)	PCA, LDA and SIMCA	Identification of fibres	2018	[104]

[1] n.a., not applicable (the study did not perform multivariate analysis). [2] n.d. number of samples not defined in the study. M-PLS, modified partial least squares regression. SECV, standard error of cross-validation. SEV, external validation error. RPD, residual predictive value. PCA, principal components analysis. LDA, linear discriminant analysis. SIMCA, soft independent modelling of class analogy. LSSVM, least squares support vector machine. PLS-DA, partial least-squares discriminant analysis. CNN, convolutional neural network. TCN, temporal convolutional neural network. PCR, principal component regression. RMSEP, root mean square error of prediction. HCA, hierarchical cluster analysis. RMSEC, root-mean-squared error of calibration. RMSECV, root-mean-squared error of cross-validation. NRS, nearest regularisation subspace. SVDD, support vector data description. KNNDD, k nearest neighbour data description. ELM, extreme learning machine. SPA, successive projection algorithm. LWA, loading weights analysis. RCA, regression coefficient analysis. CVA, canonical variate analysis. MCUVE, Monte Carlo uninformative variables elimination. SPA, successive projections algorithm. GA, genetic algorithm. MCR, multivariate curve resolution. MAE, mean absolute error. * Studies with sample sizes < 30 are generally best interpreted as proof-of-concept and may require additional large-scale, diverse validation before industrial deployment.

4.1.5. Model Validation and Application

The recommended final step is model validation which typically includes an independent set of known samples, which is usually smaller than the training set. Aljannahi and Alblooshi [82] allocated 70% of samples for training and 30% for validation, while Chen and Men [86] used an 80/20 split. Validation samples always undergo the same acquisition and pre-processing steps as the training samples. Model accuracy is further assessed by comparing predicted versus true classifications. Several studies report high accuracy rates. Chen and Lin [33] achieved 100% sensitivity and specificity in identifying natural animal fibres using PCA-LDA and SIMCA models. Chen and Men [86] developed an LSSVM model optimised with VISSA and Particle Swarm Optimisation (PSO), which provided accurate quantitative analysis of wool/cashmere blends. Aljannahi and Alblooshi [82] distinguished four synthetic fibres (acrylic, rayon, nylon, and polyester) with 97% accuracy using PCA and SIMCA, although they recommended increasing the training set size and incorporating additional analytical methods. Conversely, Davis and Busch [77] observed reduced accuracy when the number and diversity of fibres increased; their SIMCA model achieved only 62% and 24% correct classification for cotton and silk, respectively, among six fibre types. The lack of sample standardisation regarding origin, finishing, weave, and dye content likely contributed to this limitation. Model accuracy appears to be highly dependent on four key factors: (i) the size and diversity of the training set, (ii) the quality of spectral pre-processing, (iii) the modelling technique or combination of techniques employed, and (iv) the spectroscopic method(s) used for data acquisition.

4.2. The Role of Chemometrics in Textile Fibre Discrimination

The integration of chemometric techniques with vibrational spectroscopy has emerged as a powerful approach for the characterisation and classification of textile fibres. Given the multivariate nature of spectral data, chemometrics plays a critical role in extracting relevant information and developing predictive or classification models, enabling non-destructive, rapid, and accurate assessment of fibre composition and quality. Table 4 organises studies by fibre type, distinguishing those focused on natural fibres, synthetic fibres, and mixed compositions. Regardless of fibre origin, spectroscopy combined with chemometrics has been successfully applied to discriminate fibres in both single-fibre and blended fabrics. These methods have also facilitated the prediction of fibre properties, such as diameter and quality indices, and enabled discrimination based on age, dye content, or finishing treatments. Amorena et al. [47] applied Modified-PLS regression to NIR spectra for predicting the mean fibre diameter of llama fleeces, achieving strong predictive metrics (R^2, SECV, RPD), demonstrating NIR's potential in fibre quality screening. Similarly, Canaza-Cayo et al. [48] used PCA on NIR spectra to evaluate alpaca fibre quality, highlighting its ability to detect subtle spectral differences. Balbas et al. [3] compared PCA-LDA and SIMCA for classifying cotton, wool, and silk fibres under different ageing conditions. Sun and Zhou [100] showed that both Least Squares Support Vector Machine (LSSVM) and Extreme Learning Machine (ELM) accurately classified natural and synthetic fibres, with ELM offering faster computation, an advantage for regulatory applications. The choice of chemometric or machine learning model for textile fibre classification should be guided by the specific application context, balancing the trade-off between model interpretability and classification accuracy (Table 4). Classical chemometric methods such as Partial Least Squares Discriminant Analysis (PLS-DA), Linear Discriminant Analysis (LDA), and Soft Independent Modelling of Class Analogy (SIMCA) offer high interpretability, allowing practitioners to identify which spectral features drive classification decisions [105,106]. These models establish transparent mathematical relationships between input variables and classification outcomes that can be validated against established scientific principles. For applications requiring regulatory compliance, forensic investigations, or legal proceedings, these interpretable approaches are strongly recommended, as the results can be clearly explained to regulators, auditors, or legal authorities [107]. Furthermore, these methods have a longer track record in analytical chemistry and are more likely to be accepted by regulatory bodies.

Table 4. Comparison of chemometric and machine learning models for textile fibre classification.

Characteristic	**Classical Chemometrics (PLS-DA, LDA, SIMCA)**	**Machine Learning (SVM, Random Forest, ELM)**	**Deep Learning (CNN, ANN)**
Interpretability	High	Moderate	Low
Accuracy on simple datasets	High	High	High
Accuracy on complex datasets	Moderate	High	Very High
Training data requirements	Low–Moderate	Moderate	High
Computational resources	Low	Moderate	High
Regulatory acceptance	Established	Emerging	Limited
Best suited for	Quality control, forensics, regulatory compliance	Industrial screening, research	High-throughput sorting, recycling facilities

Conversely, for high-throughput industrial applications such as automated textile sorting in recycling facilities, where processing speed and classification accuracy take precedence over model interpretability, deep learning approaches including Convolutional Neural Networks (CNNs) and Artificial Neural Networks (ANNs) are more appropriate. Riba et al. [108] applied CNNs to NIR spectra for the classification of post-consumer textile waste, achieving 100% correct classification for pure fibres and 90–100% for binary mixtures. Similarly, Tsai and Yuan [109] developed a Raman-spectroscopy-based system integrating CNNs that achieved over 95% precision when categorising textiles by fibre composition, with a throughput of one piece per second. These models excel at handling complex, non-linear relationships in spectral data and can achieve superior accuracy when trained on large, diverse datasets encompassing real-world variability [110]. However, their "black-box" nature makes it difficult to explain why a particular classification was made, which may be problematic in contexts requiring traceability or auditability. It is important to emphasise that despite the growing popularity of deep learning approaches, classical chemometric methods such as PCA and PLS remain indispensable in the analytical workflow. These techniques are routinely employed for spectral preprocessing, noise reduction, and dimensionality reduction before applying more complex AI models, effectively "cleaning" the data to improve subsequent classification performance. Furthermore, for small-scale projects or exploratory studies where limited sample numbers preclude the training of data-intensive deep learning architectures, PCA and PLS-based methods offer robust and reliable classification with modest datasets, often requiring only 20–50 samples per class to build stable models, compared to the hundreds or thousands typically needed for CNN training [111,112].

Intermediate approaches, such as Support Vector Machines (SVMs), Random Forests, and Extreme Learning Machines (ELMs), offer a balance between interpretability and accuracy. These methods can handle moderate non-linearity while still providing some insight into feature importance, making them suitable for research applications and industrial quality control where both performance and understanding are valued. In practice, a hybrid strategy may be advantageous: initial model development and validation can employ interpretable chemometric methods to establish baseline performance and identify key spectral features, while more complex machine learning models can be implemented for operational high-throughput use [113]. Additionally, emerging techniques such as SHAP (SHapley Additive exPlanations) and Grad-CAM (Gradient-weighted Class Activation Mapping) can enhance the interpretability of deep learning models, potentially bridging the gap between accuracy and explainability in future applications. The integration of spectroscopy and chemometrics offers significant benefits for industrial applications, including real-time monitoring of raw materials, high-throughput screening of fibre properties, and reduced reliance on labour-intensive wet chemistry. Despite these advantages, challenges remain. Model robustness is a critical concern, especially when transferring models across instruments or sample matrices. Calibration quality depends on the representativeness and variability of the training set and on the pre-processing methods applied. Environmental factors such as humidity and temperature can also affect spectral profiles, reducing model accuracy. Furthermore, discriminating fibres with highly similar spectral features remains difficult, particularly when no chemical or morphological differences exist. In such cases, advanced multivariate models or complementary analytical techniques may be required to enhance discriminatory power.

4.3. Classification Failures: Bridging Laboratory and Real-World Applications

While numerous studies report high classification accuracies under controlled conditions, some results reveal significant limitations when models are applied to diverse, real-world samples. A notable example is the study by Davis and Busch [77], in which a SIMCA model achieved only 24% correct classification for silk and 62% for cotton when tested across six fibre types. This outcome highlights a fundamental challenge: models trained on pristine, well-characterised laboratory fibres often fail when confronted with the complexity of real-world textiles. Several factors may explain the poor performance observed for silk and other natural fibres, as summarised in Table 5.

Table 5. Factors contributing to classification failure in real-world textile samples.

Factor	Description	Impact on Spectral Analysis
Sample heterogeneity	Variation in fibre diameter, crystallinity, and morphology within and between samples	Increased spectral variability
Dyes and pigments	Presence of colourants that absorb in IR/NIR regions or cause fluorescence in Raman	Spectral interference and band overlap
Finishing treatments	Softeners, water repellents, flame retardants, antimicrobial agents	Introduction of extraneous spectral features
Fibre blends	Intimate mixing of multiple fibre types in yarns or fabrics	Overlapping spectral signatures
Ageing and degradation	Chemical changes due to light exposure, washing, or wear	Altered functional group profiles
Environmental contaminants	Dirt, oils, sweat, and other residues from use	Additional spectral noise

For silk specifically, the protein-based structure composed of fibroin and sericin can be significantly altered by degumming processes, which remove sericin and modify the spectral profile. Additionally, silk is frequently blended with synthetic fibres such as polyester to reduce cost, and these blends may not be adequately represented in training sets composed of pure fibres. The discrepancy between laboratory and real-world performance represents a critical barrier to the industrial adoption of spectroscopy-based classification systems. Most published studies employ single-fibre samples or well-defined blends with known compositions, new and unused fabrics without wear or contamination, undyed or lightly dyed samples to minimise spectral interference, and controlled environmental conditions regarding temperature and humidity. In contrast, textiles encountered in real-world recycling facilities, forensic investigations, or quality control settings are often multi-component blends with unknown proportions, heavily dyed with various colourant classes, treated with multiple finishing agents, used and contaminated with environmental residues, and aged or degraded from wear and washing. This gap underscores the need for model development strategies that explicitly incorporate real-world variability.

To improve the robustness and practical applicability of spectroscopy–chemometrics approaches, future studies should diversify training sets by including samples from multiple origins, manufacturers, and processing conditions, as well as used and aged textiles. Researchers should also incorporate dyed and treated samples, developing models that account for the spectral contributions of common dyes and finishing agents or employing preprocessing methods to minimise their interference. Furthermore, models should be tested using real-world validation sets collected from actual industrial settings such as recycling facilities or retail products rather than laboratory-prepared specimens. The transparent reporting of failure cases and analysis of their causes provides valuable insights for model improvement and should be encouraged. The exploration of machine learning approaches capable of continuous learning and model updating as new sample types are encountered may also enhance model adaptability. Finally, the establishment of publicly available spectral libraries that include real-world variability would enable benchmarking across studies and instruments, contributing to the development of more robust classification systems.

The 24% classification accuracy for silk reported by Davis and Busch [77] should not be viewed merely as a limitation but as a valuable lesson: robust fibre identification systems must be designed with real-world complexity in mind from the outset.

5. Industrial Implementation Considerations

Vibrational spectroscopy combined with chemometrics has demonstrated significant potential in laboratory settings; however, its adoption in industrial environments requires consideration of practical factors including cost, throughput, regulatory acceptance, and instrument interoperability (Table 6). The initial investment for spectroscopic equipment varies considerably depending on the technique and instrument specifications. Although the initial investment for spectroscopic instruments is higher than for conventional methods, the reduced need for consumables, faster analysis times, and non-destructive nature can result in lower long-term operational costs. Portable NIR instruments, increasingly available at lower price points (€10,000–25,000), offer a cost-effective entry point for industrial applications. Processing speed is a critical factor for industrial adoption. Conventional methods such as solubility testing and microscopy typically require 15–30 min per sample, excluding sample preparation time. In contrast, spectroscopic techniques offer significantly faster analysis. These estimates assume single-point measurements. However, when multiple replicates are required to account for fabric heterogeneity, effective throughput may be reduced.

The regulatory acceptance of spectroscopic methods for textile fibre identification is an evolving area. Currently, several ISO standards govern textile fibre analysis, such as the ISO 1833 series for quantitative chemical analysis of fibre mixtures (conventional dissolution methods); ISO 17751, which is dedicated to the determination of cashmere, wool, and other animal fibres by microscopy; and ISO 20418 for qualitative and quantitative analysis of textile fibres (includes near-infrared spectroscopy as Part 2). Notably, ISO 20418-2:2022 specifically addresses the use of near-infrared spectroscopy for textile fibre identification, representing an important step toward regulatory acceptance of spectroscopic methods. However, FTIR and Raman spectroscopy are not yet covered by dedicated ISO standards for textile analysis, although they are referenced in various ASTM (American Society for Testing Materials) and national standards for polymer identification. The absence of comprehensive international standards for all spectroscopic techniques remains a barrier to widespread industrial adoption. Industry stakeholders and researchers should collaborate to develop standardised protocols and reference spectral libraries to facilitate regulatory acceptance.

Table 6. Equipment costs, operational expenses, analysis time and throughput comparison between conventional methods and vibrational based spectroscopic ones.

	Conventional Methods (Microscopy + Solubility)	NIR	FTIR	Raman
Equipment cost * (€)	5000–20,000	15,000–60,000	25,000–80,000	40,000–150,000
Consumables per test	High (solvents, reagents)	Minimal	Minimal	Minimal
Operator training	Extensive	Moderate	Moderate	Moderate–High
Maintenance costs	Low	Low–Moderate	Low–Moderate	Moderate–High
Analysis time per sample	15–30 min	5–30 s	30–120 s	1–5 min
Estimated throughput (samples/hour)	2–4	120–720	30–120	12–60

* Costs are approximate and vary by manufacturer, configuration, and region.

A significant challenge in implementing spectroscopy-based methods is the transferability of calibration models between instruments, even those of the same type but from different manufacturers or production batches. Differences in optical components, detector sensitivity, wavelength calibration, and measurement geometry can cause spectral variations that degrade model performance. Several strategies have been proposed to address this issue; namely, (i) standardisation transfer methods- mathematical corrections that adjust spectra from a secondary instrument to match the primary instrument used for model development; (ii) robust model development– including spectral variability from multiple instruments during model calibration to create more generalizable models; (iii) universal spectral libraries—development of standardised reference libraries that account for inter-instrument variability, although such resources remain limited for textile applications; and (iv) recalibration protocols—establishing efficient procedures for model updating when instruments are replaced or serviced.

Despite these approaches, model transferability remains an active area of research. Companies adopting spectroscopic methods should anticipate the need for model validation and potential recalibration when changing instruments. Collaboration between instrument manufacturers, textile industries, and research institutions is essential to develop standardised calibration transfer protocols. Moreover, while routine spectroscopic measurements can be performed by operators with minimal training, the development, validation, troubleshooting, and updating of chemometric models require personnel with advanced expertise in both statistics and analytical chemistry—a skill set that remains scarce in many industrial settings and represents a significant barrier to widespread adoption. The literature on the industrial implementation of spectroscopy-based textile analysis remains limited. Future research should prioritise large-scale validation studies in industrial settings, comprehensive cost–benefit analyses comparing spectroscopic and conventional methods, development of international standards covering FTIR and Raman spectroscopy for textile analysis, open-access spectral databases with standardised acquisition protocols and inter-laboratory studies to assess model transferability and reproducibility.

Finally, it is important to recognise that even well-validated models can experience performance degradation over time due to instrument ageing, environmental changes, optical component drift, or variations in sample characteristics; therefore, industrial facilities should implement routine model monitoring protocols using reference samples of known composition to detect accuracy losses early and trigger recalibration when necessary, ensuring consistent and reliable fibre identification throughout the operational lifetime of the equipment.

6. Conclusions

The integration of vibrational spectroscopy and chemometric analysis represents a robust and promising strategy for the accurate, rapid, and non-destructive identification of textile fibres. Techniques such as NIR, FTIR, and Raman spectroscopy, when combined with advanced multivariate modelling, have demonstrated high potential for discriminating both natural and synthetic fibres, even in complex scenarios involving blends, dyed samples, or aged textiles. Each spectroscopic technique offers specific advantages: NIR for minimal invasiveness and suitability for in situ analysis, FTIR for detailed functional group characterisation, and Raman for superior dye detection. However, their individual limitations, including sensitivity to moisture, colour, and finishing treatments, highlight the necessity of chemometric approaches. By enabling pattern recognition, predictive modelling, and correction of spectral variability, chemometrics significantly enhances the interpretability and reliability of spectroscopic data. Despite these advances, significant gaps remain that hinder widespread industrial adoption. To bridge the gap between laboratory research and real-world application, coordinated efforts from the scientific community, industry stakeholders, and regulatory bodies are urgently needed.

The creation of a global open-access spectral library for textile fibres should be considered a priority initiative. This comprehensive database should include reference spectra for all major fibre types, acquired under standardised conditions, extending beyond pristine laboratory samples to incorporate real-world textiles including dyed, treated, aged, and blended fabrics from diverse origins. Such a resource, maintained by an international consortium, would enable researchers worldwide to benchmark their models and accelerate the development of robust identification systems. Equally important is the establishment of International Standards for Spectroscopic Fibre Analysis. While ISO 20418-2 addresses near-infrared spectroscopy, comprehensive standards covering FTIR and Raman spectroscopy remain absent. We call upon standardisation bodies such as ISO, ASTM, and CEN to develop unified protocols specifying instrument calibration, standardised acquisition parameters, recommended pre-processing workflows, minimum requirements for model validation, and guidelines for calibration transfer between instruments. The development of certified reference materials for textile fibres would further support inter-laboratory reproducibility. Additionally, large-scale validation studies in industrial settings are essential. Future research must move beyond controlled laboratory environments to validate spectroscopic methods in actual recycling facilities, quality control laboratories, and forensic units, assessing classification accuracy under real operational conditions and establishing performance benchmarks for regulatory approval. The integration of artificial intelligence and machine learning approaches, including deep learning architectures capable of continuous learning, offers significant potential for improving model robustness, though efforts must address model interpretability for regulatory acceptance.

By pursuing these strategic priorities, the research community can provide the scientific foundation for a new generation of fibre identification systems that are accurate, reproducible, and trusted worldwide. Such systems will be essential for advancing circular economy initiatives, combating textile fraud, preserving cultural heritage, and ensuring that consumers and regulators can verify textile composition with confidence.

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