JOURNAL OF MATERIALS SCIENCE 20 (1985) 859–866

Fibre orientation in machine-made paper

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Application of theories of the mechanical behaviour of machine-made paper requires statistical knowledge of the fibre orientation. Efficient experimental techniques are now available for obtaining the necessary data. These data are best represented in the form of a one-parameter distribution function. Several such distributions are offered in the literature to represent angular data. Some of the more common distributions are examined and it is shown that the wrapped Cauchy distribution is best able to predict the observed mechanical properties of a typical machine-made paper sheet.

1. Introduction

Any attempt to predict the mechanical behaviour of a machine-made paper sheet must necessarily base itself on a measured or assumed arrangement of the fibres in the sheet. For use in theories of mechanical behaviour this information, under the assumption of random fibre orientation in the plane, is best represented in the form of a probability density function $f(\theta)$. $f(\theta)\,\mathrm{d}\theta$ is the fraction of fibrous material to be found between the angles θ and $\theta + \mathrm{d}\theta$. θ is generally measured with respect to the machine direction. Most analyses have utilized the probability density function when it is represented as a Fourier series

$$\pi f(\theta) = 1 + a_1 \cos 2\theta + a_2 \cos 4\theta + a_3 \cos 6\theta + \ldots \quad (1)$$

Only cosines need be included since the distribution should be symmetric with respect to the x (machine) direction and of these only even cosines need be included since the distribution would be symmetric with respect to the y (cross) direction. The basic network theory of the elastic behaviour of paper was formulated by Cox [1] thirty years ago. He found that the four elastic constants necessary to define the in-plane linear elastic behaviour of paper can be expressed in terms of the *first two coefficients* of a cosine series expansion as follows:

$$\frac{1}{E_x} = S\frac{6-4a_1+a_2}{2+a_2-a_1^2} \quad (2)$$

$$\frac{1}{E_y} = S\frac{6+4a_1+a_2}{2+a_2-a_1^2} \quad (3)$$

$$\frac{1}{G_{xy}} = S\frac{16}{2-a_2} \quad (4)$$

$$\nu_{xy} = \frac{2-a_2}{6-4a_1+a_2} \quad (5)$$

Here E_x and E_y are the Young's moduli in the machine and cross directions respectively, G_{xy} is the in-plane shear modulus, and ν_{xy} is a Poisson ratio (the ratio of strain in the y-direction to strain in the x-direction when stress is applied only in the x-direction). S is essentially a scale factor – the axial compliance of a fibre divided by the volume fraction of fibres in a sheet. We note that the anisotropy ratio $\xi = E_x/E_y$ is given simply by

$$\xi = \frac{6+4a_1+a_2}{6-4a_1+a_2}. \quad (6)$$

The Cox model assumes that all strain energy stored in the sheet is due to axial tension (or compression) in the fibres. Since Cox's original work many other network type models for describing the mechanical behaviour of paper have been put forth. These have tried to account for, among other things, the influence of finite fibre length, bond elasticity, fibre curl, fibre bending and shear, drying stresses, out of plane effects, etc. Generally the analyses have included microstructural parameters which are difficult to measure directly and whose values can only be inferred. Such

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models might also include additional Fourier coefficients other than the two utilized in the Cox model; specifically, a_3 appears in some formulations [2]. In models for the inelastic behaviour of paper additional Fourier coefficients will almost certainly appear [3]. But it is generally accepted that the basic description of the linear elastic behaviour of a well bonded paper sheet is given by the Cox model. Indeed it has been argued, based on experimental evidence, that it is really a quite good description [4–6], except perhaps in the case of groundwood pulps [6]. Hence in considering fibre distributions we will be particularly interested in the first two Fourier coefficients because of their centrality in determining the essentials of the linear elastic behaviour.

A number of one-parameter distributions have been suggested for describing fibre orientation in an anisotropic sheet. The simplest choice would be to retain only the first cosine term in the Fourier representation of the probability density function of Equation 1; i.e. $a_1 \neq 0$, $a_2 = 0$, and all other higher Fourier coefficients are zero. This is the bimodal cardioid distribution [7, 8]. In comparing distribution functions we would like some measure of the dispersion of the distribution. We will take this, as is customary, to be the mean (or expected) value of $\cos 2\theta$ (the "2" is due to the bimodality of the distribution); we denote this measure of dispersion by ρ. $\rho = 0$ would be the uniform distribution, i.e. all fibre directions are equally likely; this is the situation (ideally) in a hand sheet. $\rho = 1$ would imply that *all* fibres are oriented in the machine direction. It is clear that generally $a_1 = 2\rho$ for any distribution. Thus the bimodal cardioid distribution has the probability density function

$$\pi f_{\mathrm{H}}(\theta) = 1 + 2\rho \cos 2\theta. \qquad (7)$$

In handling angular data one would like to find an equivalent of the normal distribution on the line. Unfortunately no one candidate can be found which has all the desirable properties of the normal distribution. The two most likely contenders are the wrapped normal distribution and the von Mises distribution [9, p.68]. The wrapped normal distribution is best represented by the Fourier series expansion of its probability density function

$$\pi f_{\mathrm{N}}(\theta) = 1 + 2 \sum_{n=1}^{\infty} \rho^{n^2} \cos 2n\theta. \qquad (8)$$

ρ is again the measure of dispersion, the mean value of $\cos 2\theta$. $a_1 = 2\rho$ of course, but $a_2 = a_1^4/8$.

The von Mises probability density function is

$$\pi f_{\mathrm{M}}(\theta) = \frac{1}{I_0(\kappa)} \mathrm{e}^{\kappa \cos 2\theta}. \qquad (9)$$

Here $I_0(\kappa)$ is the modified Bessel function of the first kind and zero order. The Fourier series form is

$$\pi f_{\mathrm{M}}(\theta) = 1 + \frac{2}{I_0(\kappa)} \sum_{n=1}^{\infty} I_n(\kappa) \cos 2n\theta \qquad (10)$$

where $I_n(\kappa)$ is the modified Bessel function of the nth order; and it is easily shown that

$$a_2 = 2(1 - a_1/\kappa) = 2(1 - 2\rho/\kappa) \approx a_1^2/4. \qquad (11)$$

This last approximation is arrived at by examining the asymptotic form of the Bessel functions and can be shown to be quite accurate for the range of as relevant to our problem. However the approximation is for visual comparison only and will not be used in calculations; as are to be calculated from Equation 10. Mardia [9, p.68] points out that these last two distributions can be made to approximate each other closely, and that they both display certain valuable characteristics of the normal distribution on a line, and further that the properties of the wrapped normal are approximately enjoyed by the von Mises distribution, and concludes that either can be chosen as an appropriate normal distribution where the final choice is essentially a matter of convenience. These two distributions play a dominant role in the study of angular random variables. However, for the particular problem at hand, i.e. describing fibre distribution in a paper sheet, we will show that these distributions are definitely not appropriate; the definitively appropriate distribution will be shown to be the wrapped Cauchy distribution given by,

$$\pi f_{\mathrm{C}}(\theta) = \frac{1 - \rho^2}{1 + \rho^2 - 2\rho \cos 2\theta} \qquad (12)$$

which has the Fourier representation

$$\pi f_{\mathrm{C}}(\theta) = 1 + 2 \sum_{n=1}^{\infty} \rho^n \cos 2n\theta. \qquad (13)$$

Thus

$$a_2 = a_1^2/2. \qquad (14)$$

Apparently the process by which the wet web is laid down favours this latter distribution. We will show that a simple transformation of variables will shift us from a uniform distribution (all directions equally likely) to the wrapped Cauchy distribution. Thus this distribution can result from a "warping" of the uniform distribution by some physical process. An extremely idealized and simplistic suggestion will be made to illustrate this.

2. Comparison of distributions

It has long been conjectured that a special relationship may exist between the in-plane elastic constants of paper [10, 11]. The implication of this conjectured relationship is that the in-plane shear modulus of a paper sheet is independent of angle with respect to machine direction [12]. The angular independence of G was first experimentally corroborated indirectly by Horio and Onogi [10]. A number of investigators [12–15] have measured the shear modulus for various papers as a function of angle to the machine direction, and found it to be essentially constant. Schulgasser [5, 6] showed that this assumption together with the Cox network model implies that knowledge of the anisotropy ratio $\xi = E_x/E_y$ determines uniquely the invariant shear modulus and the Poisson ratio of the paper, and that experimental evidence fits this determination. One cannot avoid the conclusion that the shear modulus is at least more or less independent of angle. We will now check for the invariance of the shear modulus for the several distributions which have been presented.

The variation of shear modulus as a function of angle with respect to the machine direction is given by

$$\frac{1}{G_\theta} = 4\left[\frac{1+2\nu_{xy}}{E_x} + \frac{1}{E_y}\right]\cos^2\theta\,\sin^2\theta + \frac{(\cos^2\theta - \sin^2\theta)^2}{G_{xy}}. \qquad (15)$$

It is easy to show that the maximum deviation of G_θ from G_{xy} is at $\theta = 45°$. Here we have

$$\frac{1}{G_{45}} = \frac{1+2\nu_{xy}}{E_x} + \frac{1}{E_y}, \qquad (16)$$

and using Equations 2 to 4,

$$\frac{G_{45}}{G_{xy}} = \frac{2 + a_2 - a_1^2}{2 - a_2}. \qquad (17)$$

For the wrapped Cauchy distribution the Fourier coefficients a_1 and a_2 are related by Equation 14, and the right-hand side of Equation 17 becomes identically equal to 1; hence G_θ is not dependent on the angle. This is what is experimentally observed. (It was already pointed out in [5] that invariance of G_θ implies Equation 14.) For the other distributions the right-hand side of Equation 17 is not 1. However this by no means excludes them out of hand. The experimental evidence is not precise enough to indicate that G_θ must necessarily be absolutely constant. We therefore examine to what extent G_{45}/G_{xy} deviates from unity. The results are given in Table I. For each anisotropy ratio the Fourier coefficients are calculated using Equation 6 together with the appropriate relationship between a_1 and a_2. Then Equation 17 is used to compute the G_{45}/G_{xy} ratio. We see that for the common range of anisotropy, 2 to 3, the deviation of G_{45} can be nearly 30% for the bimodal cardioid and for the wrapped normal distributions. This much deviation cannot be explained away. Andersson *et al.* [8] have already questioned the adequacy of a bimodal cardioid distribution in predicting mechanical behaviour. However the von Mises distribution deviates by no more than 15% and this could perhaps be justified in terms of the experimental results.

TABLE I Maximum deviation of in-plane shear modulus from its value with respect to the machine-direction/cross-direction axes

Anisotropy ratio, ξ	G_{45}/G_{xy}		
	bimodal cardioid	wrapped normal	von Mises
1.0	1	1	1
1.5	0.955	0.956	0.977
2.0	0.875	0.882	0.934
2.5	0.793	0.816	0.891
3.0	0.719	0.750	0.849
3.5	0.653	0.699	0.809
4.0	0.595	0.656	0.773

Recently Rigdahl *et al.* [16] used image analysis techniques to quantify the fibre orientation of a number of paper samples of nominal basis weight 10, 30 and 80 g m^{-2}. They automatically fitted the results to the von Mises distribution function by a least-squares method, i.e. they determined an appropriate value of the parameter κ. They also measured the Young's modulus of these samples in the machine and cross directions. Thus using the expressions for a_1 and a_2 in terms of κ as obtained from Equation 10 they could compare the anisotropy ratios as given in Equation 6 with the measured values. If, as we propose, the distribution function should properly be represented as wrapped Cauchy, one can determine, *ex post facto*,

TABLE II Comparison of calculated with experimental anisotropy ratios for wrapped Cauchy and von Mises distributions. Experimental data from [16]

Sample No.	von Mises parameter κ	Measured anisotropy ratio	Calculated anisotropy ratio (von Mises)	Wrapped Cauchy parameter ρ	Calculated anisotropy ratio (wrapped Cauchy)
10:1	0.91	2.99	3.31	0.383	2.898
10:2	1.01	3.16	3.76	0.411	3.156
10:3	0	1.27	–	–	–
10:4	0.37	1.64	1.64	0.179	1.618
30:1	0.99	2.82	3.71	0.406	3.103
30:2	0.92	2.93	3.37	0.385	2.915
30:3	0.23	1.34	1.36	0.114	1.355
30:4	0.30	1.48	1.48	0.147	1.483
30:5	1.11	3.06	4.1	0.437	3.423
80:1	0.88	2.59	3.19	0.374	2.820
80:2	0.87	2.65	3.14	0.370	2.791
80:3	0.14	1.38	1.21	0.070	1.206
80:4	0.22	1.58	1.34	0.108	1.335
80:5	0.94	2.97	3.42	0.391	2.969

the parameter ρ of the wrapped Cauchy distribution which would be least-square approximated by a given value of the parameter κ in the von Mises distribution. In other words one can follow the least-squares procedure backwards and determine for each κ found by Rigdahl *et al.* [16] the appropriate ρ. This procedure is given in the Appendix. In Table II are shown all the data of Rigdahl *et al.* (their Table I) together with the appropriate derived values of ρ and also the predicted anisotropy ratios when the von Mises distribution is used, and when the derived wrapped

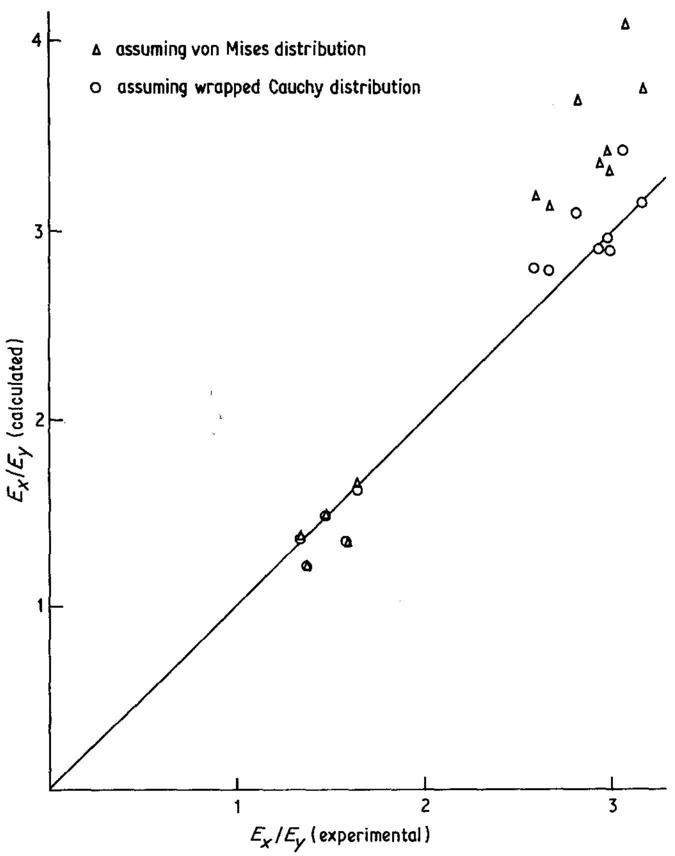

Figure 1 Comparison of calculated with experimental anisotropy ratios for wrapped Cauchy and von Mises distributions. Experimental data from [16].

TABLE III Additional comparison of calculated with experimental anisotropy ratios. Experimental data from [18]

von Mises parameter κ	Measured anisotropy ratio	Calculated anisotropy ratio (von Mises)	Wrapped Cauchy parameter ρ	Calculated anisotropy ratio (wrapped Cauchy)
0.25	1.34	1.40	0.124	1.39
0.48	1.75	1.92	0.233	1.88
1.21	4.55	4.71	0.516	4.43
1.00	3.83	3.63	0.446	3.52
1.27	5.42	4.77	0.534	4.72

Cauchy distribution is used. In Fig. 1 we compare the predicted anisotropy ratios of the von Mises distribution with those predicted by the derived wrapped Cauchy distribution. We see that the use of the wrapped Cauchy distribution brings about almost perfect correlation between the measured anisotropy ratios and the anisotropy ratios as predicted by Equation 6.

Prud'homme *et al.* [17] have described an X-ray diffraction method for determining fibre distribution. The method is indirect in that it requires that the distribution function of *fibril* orientation with respect to the individual fibre first be determined independently. The fibre distribution is then fitted by an assumed form of the distribution function. The following form was chosen to fit the fibre probability density function:

$$\pi N(\theta) = \frac{C}{C^2 \sin^2\theta + \cos^2\theta}. \quad (18)$$

For paper produced from two different pulps X-ray intensity distributions were determined and compared with those predicted when C is chosen so as to give the best fit. As pointed out by Prud'homme *et al.*, the agreement was "excellent" in one case and quite "satisfactory" in the other (see their Figs. 8 and 10), "meaning that the distribution of fibre orientation is well represented" by Equation 18. In fact one could add that for orientations of 20° and greater with respect to the machine direction the agreement is so good that looking at their figures it is hard to conceive of a better fit. At low angles of orientation with respect to the machine direction one would expect that imprecision in the choice of fibril distribution in the fibres would cause some deviation in the results, while at higher angles the precision of the final results would depend only weakly on the choice of fibril distribution. This is so since the dispersion of the fibril orientation is much much lower than that of the fibres.

The function N which was chosen is of the so-called "Hankinson" form. However with a little manipulation it can be put into the equivalent form

$$\pi N(\theta) = \frac{1 - \left(\frac{C-1}{C+1}\right)^2}{1 + \left(\frac{C-1}{C+1}\right)^2 - 2\left(\frac{C-1}{C+1}\right)\cos 2\theta}. \quad (19)$$

And now by comparison with Equation 12 it is quite clear that what we have is a wrapped Cauchy distribution with dispersion parameter $\rho = (C-1)/(C+1)$.

Before closing this section we consider the measurements made by Perkins *et al.* [18]. They compared various methods for determining fibre distribution from orientation measurements. However, in each instance, only the estimated value of the parameter κ in a von Mises distribution is reported. Six methods were considered; the values of κ found were often quite diverse. Five different papers of various anisotropy ratios were used, with the highest ratio being 5.42. They concluded that the most reliable method was the one referred to by them as "BFCL". For this method they report that the value of κ is a "maximum likelihood estimate." In a maximum likelihood approach the parameter κ is chosen such that $I_1(\kappa)/I_0(\kappa)$ equals the average of cos 2θ for all the measurements made [9, p.124]. But this average value is also an estimate of the parameter ρ in the wrapped Cauchy distribution. Hence to convert the Perkins *et al.* values of κ (which presupposes the validity of a von Mises representation) to values of ρ when the validity of the wrapped Cauchy distribution is assumed, it is simply necessary to determine ρ from

$$\rho = I_1(\kappa)/I_0(\kappa). \quad (20)$$

In Table III are shown the results reported by Perkins *et al.* The measured values of E_x/E_y are listed along with the value computed by them from their maximum likelihood estimate of κ, and

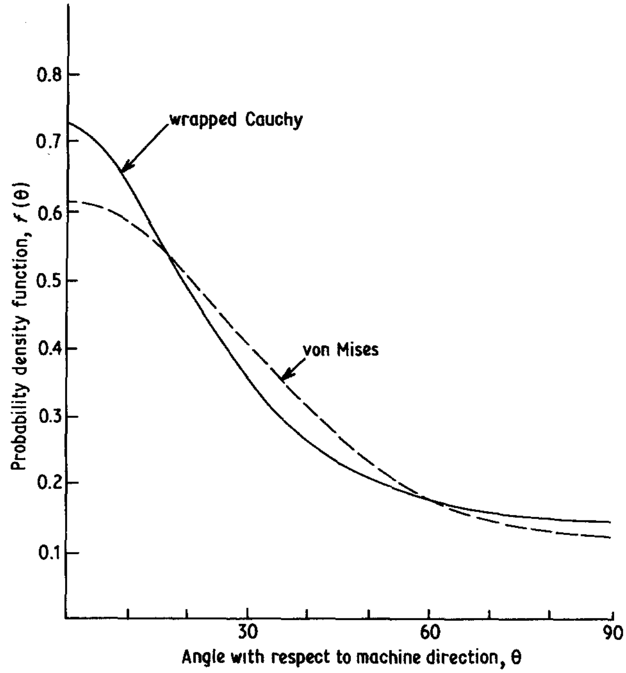

Figure 2 Comparison of the wrapped Cauchy and von Mises probability density functions for anisotropy ratio 3.

also the value of E_x/E_y computed from the reconstructed parameter ρ derived from their reported κ. The computation via ρ does not bring about much improvement of the correlation between measured and calculated values of the anisotropy ratio. In the work of Perkins *et al.* the values of a_1 and a_2 also were apparently determined by a least-squares fit to histograms, but the values are not reported in the published paper. Such values would have afforded the opportunity of directly assessing the validity of Relationship 14 between a_1 and a_2 for the wrapped Cauchy distribution offered herein, even if for only five papers, two of which showed extreme anisotropy.

3. Conclusions and discussion

The evidence in the previous section clearly points to the wrapped Cauchy distribution as being the best candidate for describing fibre distribution. We will try to give some insight into why this is so. In Fig. 2 we show the wrapped Cauchy and von Mises distributions for the instances when the anisotropy ratio as given by Equation 6 would be 3. The major difference between the curves is that the von Mises distributions puts more fibres in the orientations midway between the machine and cross directions. This would tend to lower G_{45} relatively; this showed up in Table I. We also note that the wrapped Cauchy probability density function is fairly flat from about midway between the machine and cross directions (45° in Fig. 2) until the machine direction (90°), while the von Mises function is considerably steeper in this region, as are the bimodal cardioid and the wrapped normal functions. Reported statistical data have generally shown a flat behaviour in this region ever since the first data reported by Danielson and Steenberg [19], through the measurements of Kallmes [20], and to the most recent published data [16]. Schulgasser [5] even noted that sometimes the curve seems to be increasing in the neighbourhood of 90° (the cross-direction). Wrist [21] has even measured fibre orientation distribution in the jet of a Fourdrinier machine just a few centimetres downstream of the slice and here also the characteristic flatness of the probability density function is seen.

Fig. 3 shows plots of a_2 against a_1 for the various distributions considered; also shown are lines of constant anisotropy ratio. One sees that for a given anisotropy ratio a_1 is similar for all distributions; the main variation is in a_2. At higher anisotropy ratios the variation can be significant and examining Equations 2 to 5 it is clear that the relative influence of a_2 increases for higher anisotropy ratios.

That invariance of G_θ requires the validity of Equation 14 for a simple network model had prompted Schulgasser [5] to suggest as an appropriate probability density function simply

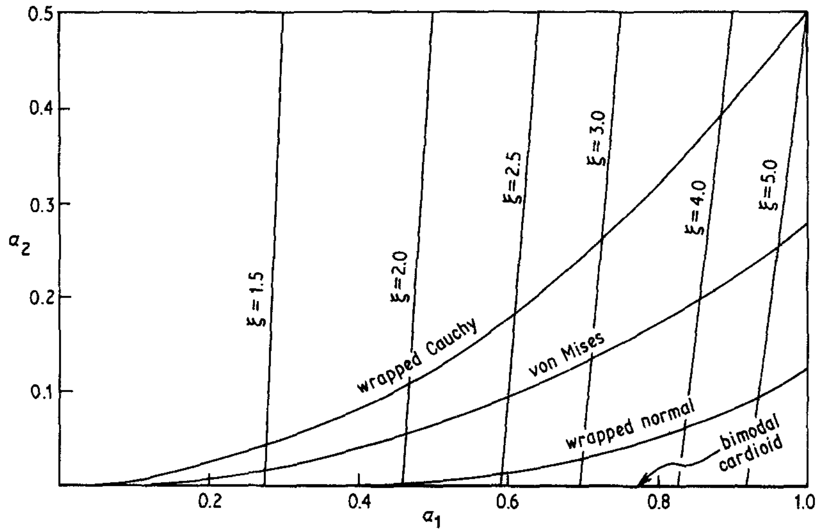

Figure 3 Relationship between the Fourier coefficients for various fibre distributions, showing lines of constant anisotropy ratio.

the Fourier representation of Equation 1 including only the first two cosine terms where the coefficients are related by Equation 14. If a least-squares fit is done with this truncated function for the extensive data of Rigdahl *et al.* [16], there is still improvement in the correlation between experimental and calculated anisotropy ratio, but it is somewhat less than for the wrapped Cauchy distribution.

We now present an heuristic rationale for the representation of fibre orientation as a wrapped Cauchy distribution. It would be folly to try to offer a model for the chaotic process, occurring in a fraction of a second, by which a fibre in the headbox approaching the slice is laid down on the moving wire with the probability of a certain orientation. But perhaps it would not be outrageous to suggest a "proto-mechanism", i.e. the fuzzy outline of a process which will lead to the observed distribution. Considering the process from above, i.e. looking down onto the plane of the paper sheet being formed, we expect that the fibre orientation in the headbox is essentially isotropic with respect to this plane. Fibres approaching the slice are accelerated very rapidly from a more or less isotropic distribution (with respect to the sheet plane) to the wire speed and almost instantly due to initial drainage and the consequent fibre interlocking are essentially frozen into their final orientation distribution. The process may be so rapid that from the isotropic state in the headbox to the anisotropic state in the sheet an individual fibre may not perform even one full gyration before settling into its permanent orientation. If so, one can ask: what is a simple distortion of a uniform fibre arrangement into an anisotropic arrangement? The most obvious would be an affine pure stretch transformation. This is explained visually as follows: consider a typical fibre as seen from above before the slice as in Fig. 4 (left-hand side). This fibre makes an angle α with the machine direction. Put a rectangular box around it of dimensions $a \times b$ as shown in the figure. Let this box distort in the process of passing through the slice according to the rule

$$a' = c_1 a$$
$$b' = c_2 b$$

where c_1 and c_2 are constants. The fibre now makes an angle θ with the machine direction (Fig. 4, right-hand side). Then

$$\tan\theta = (c_2/c_1)\tan\alpha. \qquad (21)$$

Now if we assume that α is uniformly distributed, i.e. its probability density function is simply $g(\alpha) = 1/\pi$ then one can determine the distribution of θ. Since Expression 21 is monotonic this is accomplished by a simple transformation of variables technique (see [22, p. 339ff.]) for instance). One obtains for the probability density function *exactly* the expression of Equation 18 with C replaced by c_2/c_1. So we have come full circle. The "argument" above is phrased with

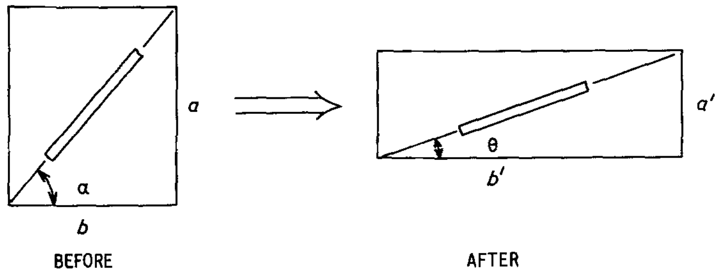

Figure 4 An affine pure-stretch transformation.

reference to a Fourdrinier machine, but would be equally applicable to laboratory-type sheet formers such as used in the investigations of references [16–18].

In conclusion, we recommend that the wrapped Cauchy distribution be adopted as a suitable one-parameter representation of fibre orientation for machine-made paper.

Appendix

If the experimental data should indeed be properly fitted by a wrapped Cauchy distribution then in seeking a least-squares fit to the von Mises distribution one is really minimizing the integral

$$\int_0^{\pi/2} [f_M(\kappa, \theta) - f_C(\rho, \theta)]^2 \, d\theta$$

with respect to κ. This is accomplished by taking the derivative with respect to κ and setting it equal to 0. Then,

$$\int_0^{\pi/2} [f_M(\kappa, \theta) - f_C(\rho, \theta)] \frac{\partial f_M(\kappa, \theta)}{\partial \kappa} \, d\theta = 0. \quad \text{(A1)}$$

Using the expressions for the von Mises and wrapped Cauchy probability density functions as given by Equations 9 and 12 we can carry out some of the integration in closed form, and after some manipulation we reduce the Condition A1 to

$$\pi I_1(2\kappa) - \pi \frac{I_1(\kappa)}{I_0(\kappa)} I_0(2\kappa) - (1 - \rho^2) \times \int_0^{\pi} \frac{I_0(\kappa)\cos\theta - I_1(\kappa)}{1 + \rho^2 - 2\rho\cos\theta} e^{\kappa\cos\theta} \, d\theta = 0. \quad \text{(A2)}$$

This equation was solved numerically for ρ as a function of given values of κ.

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Received 2 April and accepted 10 May 1984