A Statistical Model To Evaluate Fiber Bending Flexibility

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A statistical model to evaluate fiber bending flexibility

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Abstract A statistical model, that is the Kratky-Porod (KP) chain model (Kratky and Porod 1949), was first introduced to the pulp and paper field in this paper. Based on this model, a new method for characterizing the bending flexibility of fibers was developed and the pulp demand of the thinnest sheet was evaluated. Firstly, for the three types of pulps, the experimental results were compared with the KP chain model, and the resulting determination coefficients were all above 0.95, which proved that the model was feasible to be applied to these three fibers. Then, the relation between fiber bending rigidity and that of cellulosic chains inside was discussed to deduce the fiber bending flexibility. The results that have certain statistically significant were in the range of $0.6 \times 10^{11} \sim 3.5 \times 10^{11} \text{ N}^{-1} \text{m}^{-2}$, which was comparable to that of other direct methods recorded. Finally, as an application of the model, the critical concentration of paper-forming was evaluated by the fiber dimension quantified in the KP chain model. At this concentration, fiber network in one layer represented the thinnest paper in theory. To form a paper sheet with the area of 1m^2 , the minimum pulp assumption was in the range of 0.06~0.44g in theory. In conclusion, the KP chain model can be well applicable to describe the morphological characteristics of plant fibers, which will have more potential applications in the pulp and paper field.

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Introduction

The bending flexibility is one of the main intrinsic properties of the fibers. In fiber suspensions, the dimension of the flocs, which affects paper formation, is controlled by fiber properties including the flexibility (Huber et al. 2008). In the process of paper forming, as the effective bonding area of fibers varies with its flexibility, the mechanical strength of paper alters as a result (Page 2018; Yan and Li 2008). Therefore, generally speaking, the fiber flexibility has a significant influence on the paper physical and mechanical properties. It is necessary to have knowledge about the fiber flexibility in the pulp in paper industry.

Several methods have been proposed to characterize fiber flexibility, either in direct or indirect mode. Methods of flexibility coefficient and curl index are the indirect semi-quantitative ones. With the fiber theoretical length evaluated by the Bauer McNett classifier, the former is expressed as the average slope by plotting the actual length against the theoretical ones (Petit-Conil and Cochaux 1994). The latter is defined as the ratio of fiber contour length to projected length (Chandra et al. 2019). The two methods are simple and efficient with easy operation, which can be used for the laboratory control of pulp quality. However, it lacks of solid theoretical background.

Most of the fiber flexibility characterizations of an individual fiber, known as the direct methods that originates from beam bending theory in engineering mechanics. Regarding an individual fiber as an ideal elastic beam and defining the flexibility as the reciprocal of its bending stiffness, $F=1/\lambda=1/EI$, where λ is the bending stiffness, E is the elastic modulus, and I is the moment of inertia of cross-section (Rusu et al. 2001). In a simply-supported beam mode, an individual fiber was placed in the V-shaped notch across the tip of a submerged capillary tube and then drawing water into the tube (Tam Doo and Kerekes 1981, 1982). The bending force was provided by a water stream, which can be deduced by hydrodynamic theory. However, due to complex forces are exerted on fibers from the flow field, it is difficult to accurately calculate the drag force that induces fiber elastic deformation. Besides, the lower detection limit of fiber length is about 2mm, which limits its application range. In the cantilever beam model, one end of each fiber was fixed and the vertical fiber was pulled upwards by water flow

(Samuelsson 1963) or mechanical apparatus (Pettersson et al. 2017). With the aid of specialized mechanical devices (Fischer et al. 2014), the bending force and deformation of fibers can both be well investigated with high precision. Another typical approach is to measure the conformability (Yan et al. 2008 a, b). The thin wire fixed on a glass slide served as a fiber support. Wet fibers were pressed onto the wire to form a camber over it. The free-span length of the fiber is used to calculate the flexibility through small deflection beam theory. This method appears to be the simplest among the three ones as it only requires one parameter which can be measured expediently by a microscope.

As is well known, the morphology of a single fiber is nonuniform, which affects the results of the surface stiffness greatly at different test positions (Nilsson et al. 2001). Furthermore, the morphological properties of different fibers in the pulp are also different (Bergander and Salmén 2000), which can be attributed to the complex pulping process, such as the position in the plant, the growth locality of the plant, fiber separation method, etc. As a consequence, there must be large variabilities in the individual fiber measurements, indicating that mass of data should be acquired to make a statistical analysis, which seriously restricts the timeliness of some methods. In view of this, it is urgent to develop a simple and efficient method with low cost and simple operation to determine the fiber bending flexibility.

Most plant fibers have a large aspect ratio, which is consistent with the polymer chains. Therefore, it is speculated that the statistical model of the polymer chains might be applicable for fibers. Based on the KP chain model, this paper developed a new method to evaluate the fiber flexibility according to the relationship between fiber bending rigidity and that of cellulose chains inside, and further studied the influence of fiber flexibility parameters on the physical properties of paper forming.

Theoretical Model (Kratky and Porod 1949; Yamakawa and Yoshizaki 2016)

Scheme 1 The continuous mode of Kratky-Porod chain; h denotes the end-to-end vector; a denotes persistence length (Yamakawa and Yoshizaki 2016)

The Kratky-Porod (KP) chain is a coarse-grained model that describes the conformational statistics of semi-flexible polymer chains. In the continuous mode, the entire chain contour can be regarded as the continuous and differentiable curve, as shown in Scheme 1. Let L be the contour length of the entire chain, h be the end-to-end vector and s be the gyration radius vector. The mean square end-to-end distance $\langle h^2 \rangle$ can be calculated by

$$\langle h^2 \rangle = 2aL - 2a^2 \left(1 - \exp\left(-\frac{L}{a}\right) \right) \quad (1)$$

Similarly, mean-square radius of gyration $\langle R_g^2 \rangle$ can be calculated by

$$\langle R_g^2 \rangle = \frac{La}{3} - a^2 + \frac{2a^3}{L} - \frac{2a^4}{L^2} \left[1 - \exp\left(-\frac{L}{a}\right) \right] \quad (2)$$

where a is the persistence length. It is often used as the chain stiffness parameter, which is defined as the projected values of the end-to-end distance on the initial unit direction (or z axis) for an infinitely long chain.

Otherwise, in the KP model, the polymer can be regarded as the elastic wire, the bending energy of which is defined as

$$E = \frac{\lambda}{2} \int_0^L \left(\frac{\partial \mathbf{u}(i)}{\partial i} \right)^2 di \quad (3)$$

where i ($0 \leq i \leq L$) denotes the contour length of the chain, and $\mathbf{u}(i)$ denotes the unit vector tangential to the chain curve at the arbitrary point i . The bending force constant λ , which is the reciprocal of the flexibility, is defined as

$$\lambda = akT \quad (4)$$

where, k denotes the Boltzmann constant, which is equal to $1.38 \times 10^{-23} \text{J/K}$; T denotes the absolute temperature with unit K; a denotes the persistence length with unit m; the unit of λ is $\text{N} \cdot \text{m}^2$. Combined with Eq.3~6, it can be observed that the persistence length is one of the key parameters that influence the dimension and shape of the KP chain.

Materials and methods

Materials

Potassium carbonate (K_2CO_3), calcium hydroxide (NaOH), potassium iodide (KI) and iodine (I_2) were all purchased from Sinopharm Chemical Reagent Co., Ltd. Cupriethylenediamine (Cuen) was purchased from Sigma-Aldrich. All reagents were of analytical grade and used as received without further purification. The information of papermaking raw materials is listed in Table 1. Bamboo pulp was purchased from handmade paper workshop in Zhejiang, China. In addition, bast fibers of Wikstroemia and paper mulberry used were prepared by the authors with the method similar to the traditional pulping.

Table 1 Description of papermaking raw materials

Pulp	Fiber	Species	Locality (China) of growth
W-1	Wikstroemia	<i>Wikstroemia monnula</i>	Zhejiang
W-2			
W-3			
W-4			
B	Bamboo	<i>Pleioblastus amarus</i>	Zhejiang
M	Paper mulberry	<i>Broussonetia papyifera</i>	Guizhou

^a W-1, W-2, W-3 and W were taken separately from the same pulp and used in parallel experiments

Fiber separation methods

Keeping raw materials of bast fibers in boiled water for about 1h, scraping off the black impurities on the surface, then placing them in boiled alkali solution for some time. Washing them with streaming groundwater until the pH of solid pulp became neutral. At last, the fibers were obtained with a fiber disintegrator. Wikstroemia pulp was prepared in 11% (m/V) potassium carbonate solution and kept for 4 hours, while the paper mulberry pulp was obtained after 16 hours soaking in saturated lime water.

Characterization of fiber persistence length

(1) The iodine solution in high concentration needed to be prepared firstly. 4.2g potassium iodide and 0.2g iodine were mixed together. 5mL deionized water was added to the mixture drop by drop with stirring until no solid residues left, referring to ISO 9184-3.

(2) Then, pulp (4% w/v) was mixed with the iodine solution in the volume ratio of 1:1. Shaking the mixture well and storing it in the dark place.

(3) About 1ml mixture was dropwise added to the surface of a glass slide to form the thin liquid film, and then took pictures soon as possible. The imaging device was a CCD camera equipped with a plane light source at the bottom.

(4) The fiber dimension was recorded by the measuring software. The data of contour length (L) and

end-to-end length (h) of every fiber must be one-to-one correspondence. 200 or more fibers are necessary. The lower limit of detection is 0.3mm.

(5) All the data obtained from above steps were divided into about 10-15 groups at a fixed length interval. In each group, taking the average of L and h^2 respectively, and then plotting $\langle h^2 \rangle$ against L for all the groups. Finally, the persistence length a was acquired by curve fitting according to Eq. (1). The resulting values obtained in this manner have the statistically significant.

Some details require attention. The large standard deviation occurs in the range of the long fibers. It can be effectively reduced through repeated testing of such fibers to count other conformations, which can be operated by recycling the fibers after step 3 and place them in mixture, then repeating the step 3 and 4. In addition, the concentration of iodine solution will affect the results of fiber persistence length in this method. Considering that the active component of the iodine solution is easy to volatilize, it should be prepared immediately before use. It is better to test under the same ambient temperature, such as 25°C. Of course, other fiber staining solutions are also worth trying.

Fiber density measurement

Fiber density was measured according to Archimedes principle, according to the ASTM D3800–99.

The degree of polymerization measurement (Dondos and Tsitsilianis 1992; Kes and Christensen 2013)

The degree of polymerization of the pulp was measured by the viscosity method. The samples were dissolved in 0.5M Cuen at 25°C and then filtered through 0.45 μ m membranes. Combined with gradually dilute of filtrate, the efflux time of a range of concentrations was obtained through the capillary viscometer. The intrinsic viscosity $[\eta]$ was obtained according to Huggins equation. The viscosity-average degree of polymerization DP_η was calculated by

$$DP_\eta^{0.70} = 0.408[\eta] \quad (5)$$

Results and discussion

The feasibility of the KP chain theory applied in plant fibers

Most plant fibers have the large aspect ratio. Ignoring the structural details, a single fiber can be abstracted to a continuous space curve similar to the KP chain. In the KP chain model, $\langle h^2 \rangle$ conforms to the statistical distribution according to Eq. (1). Only if the experimental results of fibers are consistent with the theoretical ones, it can be proved that this model is applicable to the fibers.

In this section, $\langle h^2 \rangle$ of fibers is described as the average square distance from one end to another end of the fiber. Mass data of three different types of pulps were measured and plotted by $\langle h^2 \rangle$ against L , as shown in Fig. 1. It can be seen that the standard deviation increases with the fiber length. The reason for this is mainly because the fiber conformation increases with the length in space, but the number of data obtained in the measurement is not large enough to describe these conformations. There may be two ways to solve this problem. One is to increase the total amount of fiber tested to obtain the conformation of other fibers in the same range of length. The other is to obtain other conformations of the same fiber by the repeated test, which is equivalent to the former in theory (Matsuyama 2003).

All the data were further processed by curve fitting according to Eq. (1). As shown in Fig. 1, determination coefficients of three pulps are all above 0.95, meaning that experimental results are in good agreement with theoretical ones. The parameter of persistence length, which has the statistically significant due to the contribution of most of the fibers inside the pulp, was obtained as well. The resulting values of pulp M, W and B is 1.56 mm, 6.34 mm and 2.51mm respectively, which is basically in the same order of magnitude of the contour length as shown in Table 3, indicating that these three fibers may be the semi-flexible materials (Theo 1993). Moreover, the obvious numerical difference among three pulps demonstrates that fiber persistence length is a sensitive indicator. Parallel experiments of Wikstroemia fiber indicate that the persistence length test method shows good repeatability, as shown in Table 2.

In a word, it is feasible for the KP chain model to be applied to these three pulps. The characterization method of the fiber persistence length is simple and reliable with high sensitivity and precision. In addition, according to Eq. (4), the persistence length may be related to its bending

flexibility that influences the paper performance, therefore, it is worth further research.

Table 2 Comparison of persistence length of Wikstroemia fiber

Pulp	Persistence length $a(\text{mm})$	Standard error (mm)	R^2	Count
W-1	6.56	0.68	0.99	139
W-2	6.37	0.50	0.99	209
W-3	6.34	0.46	0.99	322
W-4	6.02	0.39	0.99	670
Average ($\bar{a}$)	6.32

Fig. 1 The application of the KP model in three pulps named Wikstroemia (a), Bamboo (b) and Paper mulberry (c) with standard deviation and the results of the persistence length with standard error (d).

The relation between fiber bending rigidity and that of cellulosic chains inside

Plant fibers are mainly composed of linear cellulose molecules which served as the skeleton of the entire fiber. An individual fiber can be considered as a bundle of cellulosic chains. The conformations of the cellulose molecules in a fiber are affected by the hydrogen bonding provided by other cellulose molecules, and other interactions provided by impurities components. Suppose that all the cellulose molecular chains take almost the same configuration as the entire fiber and locate at any position parallel to the fiber axes, thus their persistence lengths are the same that equal to that of fiber, as shown in Fig. 2a. The bending energy of a single fiber can be regarded as the contributions of all the cellulose chain accommodated inside. It should be noted that the persistence length values in this condition relate with the particular arrangement state, which is unequal to that of mono-dispersed molecular chains.

Fig. 2 The distribution of cellulose chains in the fiber (a), and the structure of the unit cell of cellulose crystal with the hexagon denotes the glucose (b)

Consider the cellulose fiber exhibiting in uniformly cylindrical shape, where the parameter of V_0 is the actual volume, L_0 is the number-average length and d is the width of fiber in the pulp. The volume of a single fiber is divided by that of cellulose chains and the maximum number of chains that accommodated in a fiber is n_1 . The persistence length of fiber and cellulose molecules inside is the same, which is expressed as a . In the cellulose chains, L_1 denotes the contour length, DP_n denotes viscosity-average degree of polymerization, l_* denotes chain unit length and $(\pi - \theta)$ denotes the bond angle. According to the continuous KP chain theory, in the case when $\theta \rightarrow 0$, the bending energy of a single cellulose chain can be approximately calculated as (Yamakawa and Yoshizaki 2016)

$$\begin{aligned}
 E_{\text{cellulose}} &= \frac{akT}{2} \int_0^{L_1} \left(\frac{\partial u(i)}{\partial i} \right)^2 di \\
 &\approx \frac{akT}{2} \int_0^{L_1} \left(\frac{\theta}{l_*} \right)^2 di \\
 &\approx \frac{akT}{2} \left(\frac{L_1 \times \theta^2}{l_*^2} \right)
 \end{aligned} \tag{6}$$

As described above, the entire fiber bending energy is the aggregate of that of all the chains inside,

$$\begin{aligned}
 E_{\text{fiber}} &\approx \sum_{j=1}^{n_1} E_{\text{cellulose}} \approx \frac{akT}{2} \sum_{j=1}^{n_1} L_1 \frac{\theta^2}{l_*^2} \approx \frac{akT}{2} n_1 \langle L_1 \rangle \frac{\theta^2}{l_*^2} \\
 &\approx \frac{n_1 akT}{2} \left(\frac{\langle L_1 \rangle \times \theta^2}{l_*^2} \right)
 \end{aligned} \tag{7}$$

where $\langle L_1 \rangle$ denotes the average contour length of the cellulose chains inside a fiber.

According to Eq. (6) and Eq. (7), the bending force constant of fiber ought to be rewritten by introduced the parameter of n_c as

$$\lambda_{\text{fiber}} \approx n_1 akT \tag{8}$$

It can be found that n_1 and a are only two factors that affect fiber bending rigidity under the same environment temperature. The characterization of a has been made as above. Otherwise, n_1 is approximately equal to the volume ratio of fiber and cellulose chain. The actual volume of fiber can be calculated directly,

$$V_0 \approx \pi \left(\frac{d}{2} \right)^2 L_0 \quad (9)$$

The volume of the cellulose chain can be estimated by crystallographic data. The volume of the chain is divided by that of the unit cell, which have the highly symmetric structure. Native forms cellulose belongs to monoclinic system with cell dimensions of $g=8.35\text{\AA}$, $q=10.3\text{\AA}$, $v=7.9\text{\AA}$ and $\beta=84^\circ$ (Meyer and Mish 1937). As shown in Fig. 2b, the axial length of the cell is the contribution of two glucose units, the total number of cells in a cellulose chain can be expressed by $1/2 DP_\eta$. Besides, in the cross section of $g \times v$, one cell can accommodate two chains to go through, which can be calculated by “ $1+1/4 \times 4$ ”. Therefore, the volume of a single cellulose molecule is given by

$$V_1 \approx \frac{(DP_\eta)}{2} \times \frac{g \times q \times v}{2} \approx \frac{1}{4} gqv(DP_\eta) \quad (10)$$

It is well known that the plant fibers are composed of cellulose molecules and impurity components. Suppose that the impurity components, such as hemicellulose and lignin, fill the skeleton of cellulose molecules and take up no additional volume. The number of cellulose molecules that can be accommodated within a single fiber can be calculated as

$$n_1 \approx \frac{V_0}{V_1} \approx \frac{\pi d^2 L_0}{gqv(DP_\eta)} \quad (11)$$

The unit of g , q , v , d and L_0 is m, and DP_η is dimensionless.

The bending force constant of fibers can be calculated by substituting Eq. (11) into Eq. (8), and the fiber flexibility can be further calculated by $F=1/\lambda$. As shown in the table 3 and table 4, the flexibility of the three fibers is in the range of $0.6 \times 10^{11} \sim 3.5 \times 10^{11} \text{ N}^{-1} \cdot \text{m}^{-2}$, the order of magnitude of which is comparable with that of other methods reported in literature, indicating that our method is feasible to evaluate the fiber flexibility. According to Eq. (8), the persistence length, which has the statistical significance, is the parameter of fiber bending rigidity. Hence, for the fiber flexibility defined in our method, it is not within the property of an individual fiber but the results with the statistical significance. In addition, our method is easy to use through the low cost conventional laboratory instruments, making it more practical to be implemented into various laboratories as well as production lines.

This section provides a new possibility to evaluate fiber flexibility. There are some details needed to be optimized in the future. For example, to calculate the total amount molecules n_1 , the cavity structure of the fiber and the amorphous structure of the cellulose molecule may be also taken into account, in spite that only about one or two orders of magnitude differences with the existing results.

Table 3 Bending flexibility of three pulps

Pulp Parameter	B	W	M
$d(\mu\text{m})$	8	10	17
$L(\text{mm})$	1.60	3.68	5.48
$a(\text{mm})$	2.51	6.32	1.56
DP_η	1978	3238	9469
$n_c (\times 10^{11})$	2.8	6.1	8.8
$\lambda (\times 10^{-12} \text{N.m}^2)$	2.9	16.0	5.7
$F (\times 10^{11} \text{N}^{-1} \cdot \text{m}^{-2})$	3.5	0.6	1.8

Table 4 Comparison of bending flexibility of different methods

Pulp	Bending flexibility ($\text{N}^{-1} \cdot \text{m}^{-2}$)	References
Wood	$0.01 \times 10^{11} \sim 0.3 \times 10^{11}$	Fischer et al. 2014
Wood	$1.8 \times 10^{11} \sim 378 \times 10^{11}$	Pettersson et al. 2017
Wood	$0.7 \times 10^{11} \sim 73.7 \times 10^{11}$	Yan and Li 2008
Wood	$1.1 \times 10^{11} \sim 2.2 \times 10^{11}$	Huber et al. 2008
wood	$0.4 \times 10^{11} \sim 6.3 \times 10^{11}$	Tam Doo and Kerekes 1981
Bamboo	3.5×10^{11}	This work
Wikstroemia	0.6×10^{11}	This work
paper mulberry	1.8×10^{11}	This work

Influence of fiber morphology on paper forming

The KP chain model can be applied not only to evaluate the flexibility of the fiber, but also to estimate the minimum pulp demand of paper-forming. The polymer contact concentration (De Gennes 1980) is the intermediate state among the dilute and semi-dilute phase, which is applied to the suspension of fibers, as shown in Fig. 3a. Following the same idea, the condition that the fibers contact closely without overlap is defined as the critical concentration of paper forming, and the corresponding fiber network in one layer represents the thinnest paper in theory (Fig. 3b). In this section, the influence of the fiber morphological characteristics on the critical concentration of paper forming was studied by the contact concentration theory combined with the KP chain model.

Fig. 3 Schematic diagram of fiber critical concentration (a) and forming the theoretically thinnest paper (b)

Suppose that the pulp suspension is composed of homogeneous fibers with diameter d and length L_0 . Let $\langle R_g^2 \rangle$ be the mean-square radius of gyration with the meaning of the average distance between segments in a given conformation of a fiber and the fibers' center of mass. Consider the occupied space of the fiber in the suspension as the three-dimensional sphere, the radius r of which defines as

$$r \approx \langle R_g^2 \rangle^{1/2} \quad (12)$$

The occupied volume of a single fiber V_2 can be estimated as

$$V_2 \approx \frac{4}{3} \pi (r)^3 \quad (13)$$

As shown in Fig. 3a, under the critical concentration, all the fiber spheres are arranged in close-packing. Thus, the volume concentration C^* can be deduced by the ratio of actual volume (Eq. 10) to occupied volume (Eq. 13), that is

$$C^* \approx \frac{V_0}{V_2} \approx \frac{3L_0d^2}{16r^3} \quad (14)$$

Substituting Eq. (2) and Eq. (12) into Eq. (14) and performing the integration, we obtain

$$C^* \approx \frac{3L_0d^2}{16} \left[\frac{L_0a}{3} - a^2 + \frac{2a^3}{L_0} - \frac{2a^4}{L_0^2} + \frac{2a^4}{L_0^2} \exp\left(-\frac{L_0}{a}\right) \right]^{\frac{3}{2}} \quad (15)$$

It was found that the critical concentration is directly related to the fiber morphological parameters, that is the contour length, width and persistence length. The critical mass concentration can also acquire, that is, $C_1^* = \rho_0 \times C^*$, where ρ_0 represents fiber density. When the fiber spheres are arranged in one layer in the critical concentration, the forming network of fibers can be regarded as the theoretically thinnest paper sheet, as shown in Fig. 3b. Assume that the surface area of a thinnest sheet is Y , the mass demand of the pulp m^* can be required

$$m^* \approx (2r)C_1^*Y \quad (16)$$

Combined with Eq. 12~16, it can be seen that the KP chain model, which describes the fiber dimension in suspension, serves as a bridge to link the fiber morphology with the papermaking technology. Critical concentration and minimum pulp demand can be calculated through the above equations, as shown in the Table 5. To form a paper sheet with an area of 1m^2 , the theoretically minimum consumption of the three pulps is in the range of 0.06-0.44g, which is far lower than the actual pulp demand of paper-forming. According to Eq. (16), the pulp demand is positively correlated with the critical concentration. When the pulp concentration is higher than the critical concentration, the fibers in the suspension begin to overlap. The higher the pulp concentration deviates from the critical concentration, the higher the degree of overlapping of fibers inside may be. Assume the paper is formed under the same concentration, there should be more overlaps for the Wikstroemia pulp due to its minimum critical concentration, which should exert influence on the suspension properties of the pulp and the physical properties of the paper. It worth for further study in the future.

Table 5 The critical concentration of three pulps

Pulp	B	W	M
Parameter			
$\rho(\text{g/cm}^3)$	1.47	1.38	1.56
$C^*(\%)$	0.016	0.002	0.012
$C^*_1(\text{g/L})$	0.23	0.03	0.18
$m^*(\text{g})$	0.20	0.06	0.44

^a To form a sheet of paper with an area of 1m×1m, the minimum pulp mass demand is m^*

Conclusions

In this paper, a new method for characterizing the fiber flexibility was developed and the pulp demand of the thinnest paper based on the contact concentration of fibers was calculated according to the KP chain model (Kratky and Porod 1949). The determination coefficients R^2 for the theoretical model to be applied to the three pulps were all above 0.95, indicating that the model could be well applicable to those pulps. The fiber persistence length obtained in this method has certain statistical significance, so does the bending flexibility. The characterization method is simple and reliable with high sensitivity and precision.

Based on the elastic energy theory, it was found that, at a given temperature, the persistence length and the total number of cellulose chains in a fiber are the only two variables that affect the fiber bending force constant. The values of the fiber bending flexibility obtained in our method were in the range of $0.6 \times 10^{11} \sim 3.5 \times 10^{11} \text{N}^{-1} \text{m}^{-2}$. It was comparable to that of other direct methods in the literature, meaning that our method is feasible to characterize the fiber flexibility.

Following the same idea of contact concentration proposed by DeGennes (DeGennes 1980), the critical concentration of paper-forming was deduced by the fiber dimension describes in the KP model. It was found that the critical concentration is directly related to the fiber morphological parameters, such as the contour length, width and persistence length. Minimum pulp demand of paper-forming can be estimated in this concentration. Therefore, the KP chain model serves as a bridge to link the fiber morphology with the paper-forming properties. In the papermaking process, as is well known, fiber morphology should be significantly controlled by raw materials and pulping technology. Therefore, this research will play an important role in raw material selection and pulping evaluation, and is expected to

be extended to the pulp suspension to reveal the flocculation mechanism of fibers.

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Date available All data generated during this study are included in this published article.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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