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PARTICLE SIEVING IN A RANDOM FIBER NETWORK

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ABSTRACT

An idealized fiber network model is developed to study particle sieving by percolation. The model is based on a Poisson line field in two dimensions, whereby the fibers are modeled as infinite length strips of finite width, while particles are modeled as circles. The probabilistic sieving problem is equivalent to percolation of disks through convex polygons of the Poisson line field. The area-based probability of retention (equivalently, percolation) is described by an equation which depends on a single non-dimensional number that is proportional to the number of fiber per unit area and the particle size. The physical meaning and the applicable range of this number are discussed. Finally, using a Monte Carlo simulation, the model is generalized to anisotropic Poisson line fields.

Keywords: Poisson line field, random fiber network, percolation, Monte Carlo simulation.
1. INTRODUCTION

The sieving of particles in a porous random structure like paper is of importance in processes such as particle retention on a paper machine forming section or in operations such as coating and printing. It also concerns the interaction of fluids and particles with finished paper products like filters, board boxes, or cement sacks. However, particle retention by the sieving mechanism is not totally clear because paper fibers constitute a very complex, anisotropic microscopic-network when formed in a sheet of paper. It is interesting to note here that even the determination of basic geometric properties of isotropic fiber structures poses formidable challenges [11].

Our goal in this paper is to report on the development of analytical and computer models that can help in analyses of retention of particles by sieving in a fiber-microstructure model. Corte and Kallmes [1, 2] were the first to set up a random geometric model of cellulose fiber networks. Theirs was essentially a germ-grain (Boolean type) model [10] in two dimensions (in the plane of paper), in which fibers were modeled as finite rectangular elements. They defined the structure of paper as “the geometric arrangement of fibres and interfibre spaces in the sheet.” Soon thereafter, several characteristics of a planar, isotropic Poisson line field were investigated in considerable detail by Miles [3] and Richards [4]. This offered a way of modeling paper via a network of infinitely long fibers and it is adopted in the present study as well. While the assumption of infinite fibers is a rather strong idealization, the model gives closed form expressions for probability distributions of several basic characteristics (e.g., pore size) and lends itself much more easily than the finite fiber model, to computer simulations of such properties. Using a computer simulation we can also generalize it to anisotropic fiber orientations in paper.
2. MODEL FORMULATION

Fibers are initially taken as infinitely long, straight cylinders with no internal fibril structure. In projection onto an $x,y$-plane, fibers become strips of width $d_f$, with their axes being lines of the Poisson line process. In the following we work with a construction in a polar-coordinate system $(p, \theta)$, whereby a line, represented by a Hesse normal form

$$x \cos \theta + y \sin \theta = p \quad (1)$$

is specified by a distance $p$ from the origin of the $x,y$-system and an angle $\theta$ that the foot of the perpendicular to the line makes with the positive $x$-axis, Fig. 1. The $\theta$-angle range is from 0 to $2\pi$ and the $p$-distance range is from 0 to $R$. In other words, a set of randomly generated points in the $p, \theta$-plane is transformed into the $x,y$ plane, thus constituting a realization of independent random secants within the simulation window of diameter $D_w (= 2R)$. With $\theta$ being a uniform random variable, this is known as an “isotropic Poisson line field” [3-5], and effectively, a Poisson point process in the $p, \theta$ plane of intensity $\lambda$ (Fig. 1a) leads to a Poisson line field (Fig. 1b). The number of randomly generated fibers is $N_f$; these fibers form what is called a “single layer”.

The particles used in the retention analysis are the two-dimensional projections of spheres - that is, they are disks of diameter $d_p$. Like the fiber angle, the particle size can have any distribution function, but, without much loss of generality, it is assumed here to be causal (all particles have the same diameter) so as to simplify the sieving analysis.

It is assumed that each particle is being carried by a fluid, so that it will tend to move to the closest pore (polygon) relative to a given initial position in the simulation field. This model assumes
that there are no ionic, electrostatic forces or other means helping the retention of particles, and that all the particles will either pass or be retained by the fiber network depending on a "geometric fitting". Only the sieving mechanism leading to retention is of interest. Furthermore, our analysis assumes that the events of retention are independent of each other. Similarly, in the case of a Monte Carlo simulation, we always start with a "clean" fiber network - meaning that no pores are plugged – when sieving each new particle; this assumption corresponds to low particle concentrations.

In general, however, \( \theta \) may follow a preferential orientation distribution in the so-called machine-direction (MD), a situation relevant in the case of machine-made paper, which will be pursued at the end of our study.

3. **ANALYSIS**

3.1 **Polygon-number and area distributions**

The Poisson line field results in a mosaic of convex polygons. If \( d \) is the largest circle inscribed in a given polygon, its probability density \( f_N(d) \) follows a negative exponential distribution [3]

\[
f_N(d) = C \cdot e^{-\lambda d}
\]

(2)

In the above, \( N \) indicates that we deal with a polygon number-based density. The fiber width (or fiber diameter) \( d_f \) is constant by assumption, but, since the fiber length inside the window, \( l_f \), varies as it is the secant of a circle of diameter \( D_w \), an average fiber length \( \bar{l}_f \) must be used to estimate \( \lambda \), so that
Relation (2) gives a polygon-number density function \( f_N(d) \). It is independent of \( d_f \) - when the fiber width is increased, the diameter of the inscribed circle is reduced by the same quantity. An increase in \( d_f \) makes some polygons to close (the inscribed circle diameter goes to zero) so that the total number of polygons is reduced, but the relative distribution is virtually the same. It is equivalent to shifting the curve of \( f_N(d) \) to the left by \( d_f \), that is \( f'_N(d) = C f_N(d - d_f) \), but its normalization leads again to \( f_N(d) \). Constant \( C \) is used to normalize the function \( f_N(d) \) so that the (cumulative) probability distribution \( F_N(\infty) \) equals 1, that is:

\[
F_N(\infty) = \int_0^{\infty} C \cdot e^{-\lambda \cdot x} \cdot dx = 1
\]  

(4)

The network's ability to retain particles depends on the relative area of the polygon-inscribed circles, rather than on the number of polygon-inscribed circles itself. It is thus necessary to find an area-distribution function \( f_A(d) \). The corresponding density function \( f_A(d) \) can be calculated by counting the square of the diameter of each polygon-inscribed circle, which is proportional to its area. Consequently, it follows that

\[
f_A(d_i) = \frac{\text{Area of } d_i}{\text{Total area}} = \frac{(\pi d_i^2 / 4) \cdot f_N(d_i)}{\sum_{i=0}^{n} (\pi d_i^2 / 4) \cdot f_N(d_i)} = \frac{d_i^2 \cdot e^{-\lambda \cdot d_i}}{\sum_{i=0}^{n} d_i^2 \cdot e^{-\lambda \cdot d_i}} = C_A \cdot d_i^2 \cdot e^{-\lambda \cdot d_i}
\]  

(5)
In the above, \( A \) indicates that we deal with a polygon area-based density. Equation 5 has the form of a Gamma Distribution [6-8], that is

\[
f(x) = \frac{\lambda^k}{\Gamma(k)} x^{k-1} e^{-\lambda x}, \quad \Gamma(k) = \int_0^\infty x^{k-1} e^{-x} \, dx = (k-1)!
\]  

(6)

Noting from (6) that \( k = 3 \) (see also Fig. 2), it follows that \( \Gamma(k=3) = 2! \), while the constant to normalize (5) is \( C_A = \lambda^3/2 \), so that

\[
f_A(d) = \frac{\lambda^3}{2} d^2 e^{-\lambda d}
\]

(7)

This finding coincides with the experimental results of a study due to Eim et al [9]. They used non-woven fabrics to construct a fiber mat and then found the polygon-inscribed circles by using an image analysis technique. They concluded that their pore size data could be fitted by a Gamma distribution, but did not present an analytical expression. On the other hand, Dodson and Sampson [7] analytically reached the same conclusion for the pore size distribution based on the same concept of pore equivalent area from Corte and Kallmes [1] i.e. the polygon area \( a_h \) is proportional to the square of the average polygon-side length. Basically, in [7], since the x- and y-direction free-fiber lengths have Gamma distributions, the pore area also has a Gamma distribution.

### 3.2 The Sieving Equation

If a particle with diameter \( d_p \) enters the fiber network, the probability that it passes through a polygon-inscribed circle (hole) of diameter \( d_h \) is the same as the probability that \( d_h \) is larger than \( d_p \). This can be expressed as \( P(d_h > d_p) \) and it is equal to a cumulative distribution of \( f_A(d_h) \) for
all \( d_h > d_p \). On the other hand, a probability that a particle can be retained by the network is the probability that a polygon-inscribed circle diameter \( d_h \) is smaller than or equal to the particle diameter \( d_p \). These two probabilities can be expressed as:

\[
P\{\text{Retention}\} = P(d_h \leq d_p) = F_A(d_p) = \sum_{d_h=0}^{d_p} f_A(d_h) \tag{8}
\]

\[
P\{\text{No Retention}\} = P(d_h > d_p) = 1 - F_A(d_p) = 1 - \sum_{d_h=0}^{d_p} f_A(d_h) \tag{9}
\]

The cumulative distribution \( F_A(d_p) \) is a direct indication of the particle sieving probability, which is the final objective of this study. The area-density function (7) can be integrated to find \( F_A(d_p) \) and obtain an analytical expression:

\[
F_A(d_p) = \int_0^{d_p} f_A(x) \cdot dx = \int_0^{d_p} \frac{\lambda^3}{2} \cdot x^2 \cdot e^{-\lambda x} \cdot dx \tag{10}
\]

Upon an integration by parts, this yields

\[
P\{\text{Retention}\} = F_A(d_p) = 1 - (1 + \lambda d_p + \frac{\lambda^2 d_p^2}{2}) \cdot e^{-\lambda d_p} \tag{11}
\]

The parameters \( d_p \) and \( \lambda \) can jointly be replaced by a single "characteristic parameter" \( \varphi \) (taking values between 0 and \( \infty \)) because (11) is symmetric with respect to both of them, that is

\[
F_A(\varphi) = 1 - (1 + \varphi + \frac{\varphi^2}{2}) \cdot e^{-\varphi}, \quad \varphi = \lambda \cdot d_p = \frac{N_f}{D_w} \cdot d_p \tag{12}
\]
Henceforth, (12) will be referred to as a "retention probability equation" or a "sieving efficiency equation". The probability of retention of particles of size by sieving can be interpreted now as a function of tree parameters: the number of fibers $N_f$ in a circular area of diameter $D_w$ and the particle diameter $d_p$. Figure 3-a shows the retention of particles as a function of the number of fibers per window area and of the particle diameter.

In the context of paper, the number of fibers per unit area is proportional to the basis weight $W$ in paper. Then, the retention of particles by sieving in paper can be calculated directly from the basis weight by using the following relation [1]

$$\frac{N_f}{A} = \frac{W}{\bar{w}_f}$$

(13)

Where $W$ is the basis weight of the sample of area $A$ with $N_f$ number of fibers, and $\bar{w}_f$ is the average fiber weight. Substituting we find

$$\phi = \frac{N_f \cdot \bar{l}_f}{A} \cdot d_p = \frac{W \cdot \bar{l}_f}{\bar{w}_f} \cdot d_p$$

(14)

or $\phi = \frac{\text{basis weight} \cdot \text{average fiber length}}{\text{average fiber weight}} \cdot \text{particle diameter}$

3.3 **The Range of Interest and Use of the Sieving Equation**

Figure 4 shows a representation of six random networks, each at a different value of $\phi$. These values were calculated according to Table 1.
<table>
<thead>
<tr>
<th>Number of Fibers</th>
<th>Particle diameter</th>
<th>Window Diameter</th>
<th>φ</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>10</td>
<td>200</td>
<td>0.25</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>200</td>
<td>0.50</td>
</tr>
<tr>
<td>20</td>
<td>10</td>
<td>200</td>
<td>1.00</td>
</tr>
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<td>60</td>
<td>10</td>
<td>200</td>
<td>3.00</td>
</tr>
<tr>
<td>120</td>
<td>10</td>
<td>200</td>
<td>6.00</td>
</tr>
<tr>
<td>200</td>
<td>10</td>
<td>200</td>
<td>10.00</td>
</tr>
</tbody>
</table>

Table 1. Determination of φ for Figure 4.

It is evident from Fig. 4 that, for $\varphi < 1$, the probability of retention by sieving is almost 0%, while, for $\varphi = 10$, it is nearly 100%. In summary, the range of parameter $\varphi$, for which the sieving equation has a range of interest, can be identified as $0 \leq \varphi \leq 10$. Clearly, the value of $\varphi$ is characteristic of each network-particle system, and we propose it as a new dimensionless number.

3.4 The anisotropic case

It is noteworthy that the fiber orientation has no effect on the value of $\lambda$ (number of fibers per unit area) – it remains the same. Thus, the number of polygon-inscribed circles and their size distribution are independent of the fiber angular orientation. Interestingly, Miles [3] established this result for a polygon-number distribution of inscribed circles in an anisotropic Poisson line field. That is, his Theorem 4, “The distribution of $D$ (in-circle diameter) is negative exponential”, generalizes from the isotropic case to the anisotropic case. However, the area distribution of the polygon-inscribed circle distribution was outside the scope of that work.
In order analyze this aspect, a computer program had to be developed so as to assess the desired properties via a Monte Carlo simulation; see the appendix. Our attention is focused on an angle distribution function of the Fourier series type [12]

\[ g(\theta) = \frac{1}{2\pi} \sum_{n=0}^{\infty} a_n \cdot \cos(2n\theta), \quad 0 \leq \theta \leq 2\pi \]  

We have tried several values of the \( a_0, a_1, \) and \( a_2 \) coefficients, see Table 2. Results of the first of these cases, which, actually, is the strongest case of preferential orientation of fibers relative to the \( y \)-axis (Machine Direction (MD) in the paper science terminology) are shown in Fig. 5. In particular, Fig. 5-a presents a plot of the assumed and the simulated angle distributions so as to indicate the quality of the Monte Carlo simulation using just 200 lines. Next, Fig. 5-b plots the retention probability according to the simulation and according to our sieving equation (12). Evidently, the fit is very good; it was equally good in other cases of Table 2.

<table>
<thead>
<tr>
<th>Case</th>
<th>( a_0 )</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1/2</td>
<td>1/8</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1</td>
<td>1/4</td>
</tr>
</tbody>
</table>

Table 2. Coefficients of Equation 15.

4. CONCLUSIONS

To simulate and study the retention of particles by sieving in a fiber network, the first and most important requirement is to define the number of fibers per network area and the particle size.
The number of inscribed circles and their size distribution in a fiber network model made of infinite-length lines are independent of the fiber orientation. The pore-size distribution, based on the measurement of the polygon-inscribed circle, has a Gamma distribution that is a function of the number of fibers per unit area only.

The equation developed to predict the retention probability or the sieving efficiency of particles in a fiber network is a function of a dimensionless parameter, called \( \varphi \). This parameter, in turn, is proportional to the number of fibers per unit area and the particle size. The usefulness of the dimensionless parameter \( \varphi \) is that its magnitude provides an initial estimate of the range for which the retention by the sieving mechanism in a fiber network is either feasible or negligible.

The simulation model results and the analytical expressions developed are in agreement with physical simulation models made of wax bars resembling the fibers and marbles resembling the particles. Bearing in mind the model assumptions (cylindrical fibers, spherical particles, uniformity, etc.), the present model should be applicable to particle sieving in fiber mats. However, the degree of agreement and applicability to paper needs further study. This can probably be achieved by finding and introducing an appropriate correction factor to the model.

REFERENCES


**NOTATION**

- $a, b, c$ General coefficients
- $A$ Area
- $C$ Constant
- $d_f$ Fiber diameter
- $d_h$ Hole or pore diameter
- $d_p$ Particle diameter
- $D_w$ Window diameter
- $f(d)$ Distribution function
- $F(d)$ Cumulative distribution of $f(d)$
- $g(\theta)$ Angle distribution function
- $k$ General integer constant
- $l_f$ Fiber length
- $n$ General integer number
- $N_f$ Number of fibers
\( p \) Distance from line to coordinate origin
\( P \) Probability function
\( r \) Polygon inscribed circle radius
\( r_A \) Triangle inscribed circle
\( W \) Basis weight
\( w_l \) Fiber weight per unit length
\( \bar{w}_f \) Average fiber weight
\( x, y \) General variables

**GREEK SYMBOLS**

\( \Gamma \) Gamma distribution function
\( \varphi \) Sieving dimensionless parameter
\( \lambda \) Coverage parameter (number of lines per unit area)
\( \theta \) Orientation angle
APPENDIX A

Computer Model of Retention in Anisotropic Fiber Networks

Bearing in mind the assumptions and definitions stated for the present model, the procedure to construct the computer fiber network is as follows. First, a circular simulation window of diameter $D_w$ is defined. Then, $N_f$ lines are drawn randomly according to the transformation illustrated in Fig. 1a); each line is specified by an angle $\theta_i$ and a distance $p_i; i = 1, 2, \ldots, N_f$. The program follows a "target function", to generate a fiber orientation angle. As an example, this function generates the frequency distribution shown in the histogram on Fig. A-1, which correspond to the Poisson line field presented in Fig. 1-b. This histogram also presents the distribution of the angles generated by the program. There is a good agreement between both histograms, which means that the algorithm is following the target function closely. In this example, there are 200 lines, which constitute a layer of 200 fibers. These lines, which are expressed in a polar-coordinate system, are converted to the $x$-$y$ coordinate system by finding their respective parametric equations. All the $x$-$y$ intersection coordinates of these infinite-length lines are found, inside and outside the window, by solving the two corresponding equations for each pair of combinations. In matrix notation

$$
\begin{bmatrix}
    a_i & b_i \\
    a_j & b_j
\end{bmatrix}
\begin{bmatrix}
    x \\
    y
\end{bmatrix} =
\begin{bmatrix}
    c_i \\
    c_j
\end{bmatrix}
$$

(A-1)

This process gives $k$ ($k = N_f \cdot (N_f - 1)/2$) intersections. These intersection points are arranged to form a $2 \times k$ matrix and constitute the only information strictly necessary for subsequent calculations. The $N_f$ lines form convex polygons and each of these intersecting points is a polygon vertex.
The parameter that determines whether a disk can pass through a polygon, $P$, is the size of the largest inscribed circle, and this is what constitutes the main challenge in developing a computer program. If the polygon is a triangle, finding the inscribed circle is straightforward because there is a geometrical relation between the triangle sides ($l_1, l_2$ and $l_3$) and the radius of such a circle. Denoting a triangle’s semiperimeter by $s$, we have

$$r_a = \frac{s \cdot (s - l_1) \cdot (s - l_2) \cdot (s - l_3)}{s}, \quad s = \frac{1}{2}(l_1 + l_2 + l_3) \quad (A-2)$$

By definition, the distance from the center of the inscribed circle to each side of the triangle is constant and each side is tangent to the same circle.

If the polygon $P$ is more than three-sided, we need to consider all the possible triangles $\Delta$ formed by the extension of the polygon sides (see Fig. A-2). Then, the polygon-inscribed-circle is identified to be the smallest of all the triangle-inscribed circles: $r = \min_{\Delta} \{r_\Delta\}$. On the other hand, the radius of an inscribed circle is found using equation (A-2): this is, strictly speaking, a maximum over all circles $C$ contained within a given triangle $\Delta$: $r_\Delta = \max_{C \subseteq \Delta} \{r_C\}$. Thus, the polygon inscribed-circle is found as a solution of a saddle-point problem:

$$r = \min_{\Delta} \left\{ \max_{C \subseteq \Delta} \{r_C\} \right\} \quad (A-3)$$

Starting with the lowest $x$-$y$ coordinate vertex of each polygon, the program identifies each polygon by “walking” through its sides in a counter-clockwise manner until it reaches the starting vertex. Each polygon side is transformed into a vector form by finding the difference between its
ending coordinates, $x_j, y_j - x_i, y_i$. The vector’s cross-product ($\vec{v}_i \times \vec{v}_j$) properties are used to find and keep the counter-clockwise direction.
Random generation of $\rho$ and $\theta$

Poisson line field

Figure 1-a. Generation of the Poisson Line Field

Figure 1-b. Poisson Line Field of 200 fibers
Figure 2. Gamma Distribution Function

\[
\Gamma(k) = \int_0^\infty x^{k-1} e^{-x} \, dx = (k - 1)!
\]
Figure 3-a. Probability of Particle Retention by Sieving as Function of $\phi$

Figure 3-b. Probability of Particle Retention by Sieving as Function the number of fibers per window-area and particle diameter
Figure 4. Samples of Particle-Fiber Networks for different values of $\phi$. 
Angle Frequency Distribution

\[ g(\theta) = \frac{1}{2\pi} [1 + 1 \cdot \cos(2 \cdot \theta)] \]

Figure 5-a. Fiber-Angle Orientation

Particle Retention in an Oriented Fiber Network

Figure 5-b. Sieving Efficiency for an Anisotropic Case
Figure A-1. Fiber Orientation According to the Angle Distribution Function

\[ g(\theta) = \frac{1}{24} \left[ 1 + \frac{1}{2} \cos(2 \cdot \theta) + \frac{1}{8} \cos(4 \cdot \theta) \right] \]

Figure A-2. Polygon Inscribed Circle