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Boundary length and internal surface area measurements in porous materials with elliptical pores

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Formulae are derived for the stereological determination of boundary length per unit area, B_A, and surface density, S_V, in materials with elliptically shaped pores. These relationships are valid for two-phase solids with orthotropically distributed internal surfaces (surfaces that can be mapped onto an ellipsoid). Maximum and minimum mean intercept length measurements in a plane are needed to calculate B_A. Mean intercept length measurements in the three principal directions of porous symmetry are necessary to calculate S_V. If the principal directions are not known they can be found by calculating the eigenvectors of a second rank tensor called the mean intercept length tensor. In a material with a transversely isotropic distribution of internal surfaces (surfaces that can be mapped onto a spheroid), mean intercept length measurements along and transverse to the axis of symmetry are needed to calculate S_V.

Nomenclature

S_V Surface density (internal surface area divided by test volume) ($mm^2 mm^{-3}$).
S/V Internal surface area divided by volume of voids ($mm^2 mm^{-3}$).
B_A Profile boundary length divided by test area ($mm\ mm^{-2}$).
B/A Profile boundary length divided by area of voids ($mm\ mm^{-2}$).
P_L Number of profile boundaries intersected by a test line divided by the length of the test line (mm^{-1}).
MIL Mean intercept length $1/P_L$ (mm).
MPC Mean chord length of the pores within a test area in a given direction (mm).
MSC Mean chord length of the solid matrix within a test area in a given direction (mm).
L_L Lineal solid fraction (length solid passed through by a test line divided by the total length of the test line).
A_A Solid area fraction (fraction of solid area per test area).
V_V Solid volume fraction (fraction of solid volume per test volume).

1. Introduction

Quantitative stereology is the characterization of three dimensional geometries within a specified volume from measurements made on a plane (or several planes) cut through that volume. Stereological measurements include measurement of volume, surface, orientation, and number of features. Basic stereological relationships are compiled by Underwood [1], DeHoff and Rhines [2], and Elias [3]. In this paper we are concerned with the stereological relationship between lineal measurements and internal surface in porous materials with elliptical pores.

Internal surface area is an important measurement in the study of many engineering and biological materials. Internal surface area is a function of pore size. This property along with porosity are major factors responsible for the mechanical property characteristics of porous engineering materials. In many biological systems function depends upon the rate at which activities occur at a surface. The overall rate of function in these systems is surface-dependent. Therefore, from a physiological standpoint, surface area measurements are very meaningful. Some surface-dependent functions are remodelling of bone, gas transfer in the lung, and filtration in the glomeruli of the kidney.

In materials with isotropic internal surface, meaning that the normals to the measured surface are randomly distributed, surface density, S_V, can be found easily by a simple point count on sections of the material. The relationship between S_V and the lineal point count, P_L, is derived in [1–3].

$$S_V = 2P_L \tag{1}$$

Elias [3] presented a simple model for measuring S_V in isotropic porous materials. He assumed that if one distribution of internal surfaces is isotropic, surface elements can be rearranged onto the surface of a sphere. Furthermore, he asserted that this model is correct for the internal surface area of a porous material whether the voids are spherical or not, as long as they are randomly arranged in space. Whitehouse [4] restated this model and showed that if an isotropic porous material underwent linear expansion or contraction in a given direction, surface elements could be mapped onto a spheroid. In a similar fashion, we will assume that if an isotropic porous material undergoes linear expansion or contraction in two (or three) orthogonal directions, surface elements can be rearranged upon the surface of an ellipsoid. We will also assume that the dimensions of this ellipsoid can be related to stereological measurements along its axes of symmetry.

The analog to surface density in two dimensions is boundary length per unit area, B_A. In isotropic porous materials B_A is proportional to P_L and therefore proportional to S_V [1–3]. However if the isotropic relationship is extended to anisotropically porous materials, significant errors can result. Whitehouse [4] analysed the special cases of isotropic porous materials which have become anisotropic as a result of linear expansion or contraction in a given direction. Such materials have porous symmetry that has one preferred direction and can be referred to as transversely isotropic. He determined, numerically, the proportionality constant between S_V and B_A for models with varying degrees of directionality or anisotropy. The results showed that in materials with transversely isotropic surfaces, this proportionality constant is highly dependent on the plane of measurement and degree of anisotropy.

The derivations presented in this paper are based on the assumption that many anisotropic porous materials have porous symmetry that is ellipsoidal. For example, this was shown to be true in cancellous bone by Whitehouse [5], and Harrigan and Mann [6]. Whitehouse found that mean intercept lengths measured in various directions in a plane of cancellous bone correlated well with the equation of an ellipse. Harrigan and Mann furthered this work by showing that similar elliptical symmetries existed in each of three orthogonal planes. They noted that these ellipses were projections of an ellipsoid and, by the theory of quadratic forms, could be represented as a second rank tensor. They called this tensor the mean intercept length tensor (see [6] for a description of the stereological measurement of the mean intercept length tensor). The eigenvectors of the tensor represent the directions of the axes of symmetry in this type of anisotropic porous material. Because the 3-dimensional porous symmetry is ellipsoidal, it can be referred to as orthotropic. In this type of porous material, surface elements can be mapped onto an ellipsoid.

2. B_A measurements

In materials with isotropic porous symmetry, B_A is proportional to a linear point count.

$$B_A = \frac{\pi}{2} P_L \tag{2}$$

In materials with anisotropic porous symmetry, P_L varies as a function of the direction of measurement. If the porous symmetry is assumed to be ellipsoidal, a plane cut through the materials will have a boundary profile that is, in general, elliptical. The inverse of P_L, called mean intercept length, is a more meaningful measurement because it is proportional to the average pore dimensions within a test area. It is assumed that the average pore symmetry is elliptical so the average pore dimensions are those of an ellipse. The radii of this ellipse, a and b, are related to mean intercept lengths along the principal axes, MIL_1 and MIL_2, as follows:

$$a, b = \frac{4}{\pi}(1 - A_A) MIL_1, MIL_2 \tag{3}$$

(derived in Appendix A). The total profile boundary length divided by the area of voids is equal to the boundary length of an ellipse of average pore dimensions divided by its area. The boundary length of an ellipse, with principle radii a and b, is expressed as an elliptic integral of the second kind [7].

$$B = 4 \int_0^{\pi/2} [a^2 - (a^2 - b^2) \sin^2\theta]^{1/2} \, d\theta \tag{4}$$

A common approximation of elliptical boundary length is found in [8]:

$$B \simeq 2\pi[\tfrac{1}{2}(a^2 + b^2)]^{1/2} \tag{5}$$

Boundary length divided by the area of an ellipse, B/A, is

$$B/A = B/(\pi ab) \simeq 2[\tfrac{1}{2}(a^{-2} + b^{-2})]^{1/2} \tag{6}$$

Combining Equations 3 and 6 gives:

$$B/A \simeq \frac{\pi}{2(1 - A_A)} [\tfrac{1}{2}(MIL_1^{-2} + MIL_2^{-2})]^{1/2} \tag{7}$$

B_A is proportional to B/A by the areal porosity which is a function of the solid area fraction, A_A.

$$B_A = \frac{B}{A}(1 - A_A) \tag{8}$$

Therefore, by combining the above equations,

$$B_A \simeq \frac{\pi}{2} [\tfrac{1}{2}(MIL_1^{-2} + MIL_2^{-2})]^{1/2} \tag{9}$$

The result reduces to Equation 2 when $MIL_1 = MIL_2$. Principal mean intercept lengths, MIL_1 and MIL_2, must be known to calculate B_A. If the axes of porous symmetry are known, these measurements can be made directly. However, if the axes of symmetry are not known, mean intercept lengths must be measured in various directions within the test area to fully characterize the orthotropic porous symmetry in a plane. Mean intercept lengths measured at various angles, θ, are fitted to the equation of an ellipse [6].

$$A_{xx} \cos^2\theta + A_{yy} \sin^2\theta + 2A_{xy} \cos\theta \sin\theta = \left(\frac{1}{MIL(\theta)}\right)^2 \tag{10}$$

From the coefficients A_{xx}, A_{yy} and A_{xy} the principal mean intercept lengths can be determined.

$$MIL_1 = \left\{\frac{(A_{xx} + A_{yy})}{2} - \left[\frac{(A_{xx} - A_{yy})^2}{4} + A_{xy}^2\right]^{1/2}\right\}^{-1/2} \tag{11}$$

TABLE I Boundary length per area B_A and mean intercept length MIL data for cancellous bone specimens

Specimen No.	Measured B_A (mm^{-1})	Maximum MIL (mm)	Minimum MIL (mm)	B_A (Equation 9) (mm^{-1})
1	2.767	0.579	0.471	3.039
2	1.889	1.073	0.706	1.883
3	2.097	0.974	0.530	2.386
4	1.462	1.074	0.946	1.565
5	2.194	0.822	0.513	2.551
6	2.697	0.736	0.498	2.692
7	2.573	0.797	0.527	2.528
8	3.212	0.565	0.435	3.222
9	2.187	0.898	0.582	2.274
10	2.625	0.690	0.539	2.615
11	3.505	0.468	0.417	3.566
12	1.322	1.630	0.851	1.472
13	1.718	0.922	0.835	1.795
14	1.259	1.686	1.141	1.175
15	1.926	1.031	0.730	1.865
16	1.496	0.997	0.956	1.601
17	1.844	1.312	0.812	1.609
18	1.633	1.127	1.010	1.477
19	1.453	1.329	1.074	1.330
20	1.459	1.595	1.137	1.200
1	3.269	0.686	0.399	3.219
2	3.274	0,.660	0.453	2.972
3	3.198	0.762	0.390	3.199
4	3.676	0.721	0.371	3.368
5	3.076	0.682	0.450	2.959
6	3.032	0.646	0.451	3.005
7	3.439	0.821	0.385	3.185
8	3.650	0.752	0.348	3.518
9	2.681	0.861	0.531	2.459
10	3.225	0.835	0.369	3.292
11	2.967	0.864	0.353	3.396

$$MIL_2 = \left\{\frac{(A_{xx} + A_{yy})}{2} + \left[\frac{(A_{xx} - A_{yy})^2}{4} + A_{xy}^2\right]^{1/2}\right\}^{-1/2} \quad (12)$$

3. Experimental measurements of B_A

Sections of cancellous bone from both a bovine and a human femoral condyle were analysed stereologically on an automated microstructural analysis system. MIL_1, MIL_2 and B_A were measured and are given in Table I. The results are shown in Fig. 1. The calculated values for B_A, using Equation 9, compared to the measured values very well ($B_{Acal} = 0.07 + 0.97 B_{Ameas}$; $r = 0.971$).

4. S_V measurements

This analysis is designated to materials, like cancellous bone, which have elliptical porous symmetry. Furthermore, it is assumed that within a given volume of such a material, surface elements can be rearranged upon an ellipsoid which represents the average dimensions of all pores in that volume. The relationship between the radii of the ellipsoid, a, b and c, and the principal mean intercept lengths, MIL_1, MIL_2 and MIL_3, is derived in Appendix B.

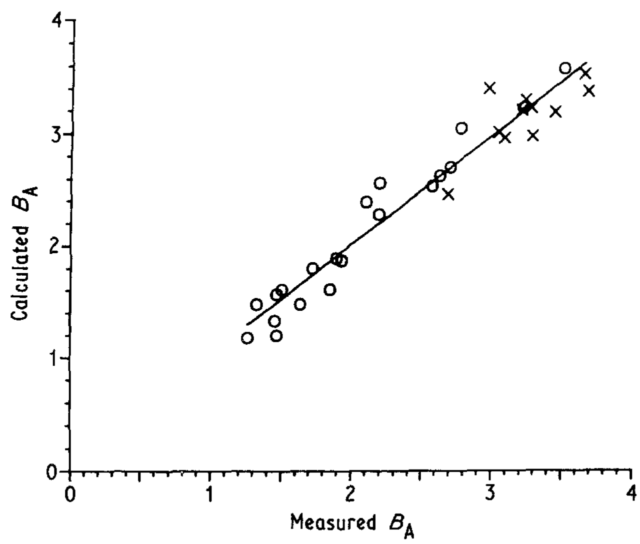

Figure 1 Comparison between B_A calculated using Equation 9 and B_A measured in cancellous bone specimens from a femoral condyle. o, data from human bone; ×, data from bovine bone.

$$a, b, c = \tfrac{3}{2}(1 - V_V)MIL_1, MIL_2, MIL_3 \quad (13)$$

The surface area of an ellipsoid, with principal radii a, b and c, is expressed as an elliptic integral [9].

$$S = 2\pi c^2 + 2\pi ab \int_0^1 (1 - k_1 k_2 u^2) \times [(1 - k_1 u^2)(1 - k_2 u^2)]^{-1/2}\, du \quad (14)$$

$$k_1 = \frac{(a^2 - c^2)}{a^2}$$

$$k_2 = \frac{(b^2 - c^2)}{b^2}$$

The solution to this equation requires restrictions on the constants, k_1 and k_2, such that no single analytical solution exists for all values of a, b and c. Therefore, a closed-form approximation was derived empirically. The resulting approximate equation is

$$S \simeq \frac{4\pi}{3}(1 - e)\, abc\, (\{\tfrac{1}{2}[a^{-2} + \tfrac{1}{2}(b^{-2} + c^{-2})]\}^{1/2} + \{\tfrac{1}{2}[b^{-2} + \tfrac{1}{2}(c^{-2} + a^{-2})]\}^{1/2} + \{\tfrac{1}{2}[c^{-2} + \tfrac{1}{2}(a^{-2} + b^{-2})]\}^{1/2}) \quad (15)$$

$$e = 0.0339\{1 - \exp[0.42(1 - a/c)]\} + 0.083\{1 - \exp[0.25(1 - b/c)]\}$$

$$\text{where } a > b > c$$

Surface areas calculated using this formula are accurate to within 1% for all values of a, b and c with the restriction that $a > b > c$.

Total surface area divided by the volume of voids, S/V, within a test volume, is assumed to be the same as the surface area of the ellipsoidal model divided by its volume. The radii of this ellipsoid, a, b and c, can be calculated from MIL measurements using Equation 13 and

$$S/V = \frac{S}{(4\pi/3)abc} \quad (16)$$

Surface density, S_V, is proportional to S/V by the volumetric porosity which is a function of the volume fraction, V_V.

$$S_V = \frac{S}{V}(1 - V_V) \quad (17)$$

By combining Equations 13, 15, 16 and 17, S_V is expressed as a function of the principal mean intercept lengths.

$$S_V \simeq \tfrac{4}{3}(1 - e)\, (\{\tfrac{1}{2}[MIL_1^{-2} + \tfrac{1}{2}(MIL_2^{-2} + MIL_3^{-2})]\}^{1/2} + \{\tfrac{1}{2}[MIL_2^{-2} + \tfrac{1}{2}(MIL_3^{-2} + MIL_1^{-2})]\}^{1/2} + \{\tfrac{1}{2}[MIL_3^{-2} + \tfrac{1}{2}(MIL_1^{-2} + MIL_2^{-2})]\}^{1/2}) \quad (18)$$

$$e = 0.0339(1 - \exp\{0.42[1 - MIL_1/MIL_3)]\}) + 0.083(1 - \exp\{0.25[1 - MIL_2/MIL_3)]\})$$

where $MIL_1 > MIL_2 > MIL_3$. The result reduces to Equation 1 when $MIL_1 = MIL_2 = MIL_3$. Mean intercept lengths in the three principal directions must be measured to calculate S_V in a material with orthotropic porous symmetry. If the principal directions of porous symmetry are not known, they can be found by calculating the eigenvectors of the mean intercept length tensor described by Harrigan and Mann [6]. Briefly, the mean intercept length tensor is measured by making mean intercept length measurements in various directions on three orthogonal planes within a test volume. Mean intercept length measurements in a given plane (designated the 1–2 plane) can be curve fit to the following equation [6]:

$$A_{11}\cos^2\theta + A_{22}\sin^2\theta + 2A_{12}\sin\theta\cos\theta = [1/MIL(\theta)]^2 \quad (19)$$

In the other two orthogonal planes

$$A_{22}\cos^2\theta + A_{33}\sin^2\theta + 2A_{23}\sin\theta\cos\theta = [1/MIL(\theta)]^2 \quad (20)$$

$$A_{33}\cos^2\theta + A_{11}\sin^2\theta + 2A_{31}\sin\theta\cos\theta = [1/MIL(\theta)]^2 \quad (21)$$

where A_{ij} are components of the mean intercept length tensor. The eigenvalues of this tensor are

$$\begin{matrix} (1/MIL_1)^2 & 0 & 0 \\ 0 & (1/MIL_2)^2 & 0 \\ 0 & 0 & (1/MIL_3)^2 \end{matrix} \quad (22)$$

$$MIL_1 > MIL_2 > MIL_3$$

MIL_1, MIL_2 and MIL_3 are the mean intercept lengths in each of the three principal directions.

5. Discussion

In general, stereological measurements must be made on three orthogonal planes to determine MIL_1, MIL_2 and MIL_3 in orthotropically porous materials. However, if the axes of porous symmetry are known, measurements on two planes of symmetry are sufficient.

There are two distinct cases of transversely isotropic porous symmetry. The first is when surface elements can be mapped onto an oblate spheroid ($MIL_1 = MIL_2$). The second is when surface elements can be mapped onto a prolate spheroid ($MIL_2 = MIL_3$). If a material has transversely isotropic porous symmetry, and the axis of symmetry is known, measurements on only one plane, which includes the axis of symmetry, is necessary for surface area calculation.

This analysis was directed toward porous materials with elliptical pores, however, the results are general to all two-phase materials with internal surfaces that can be rearranged onto an ellipsoid.

6. Conclusions

Closed formed equations have been found for boundary length per area, B_A, and surface density, S_V, for porous materials with elliptical pores. B_A and S_V are solely functions of mean intercept length measurements along the axes of porous symmetry.

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Appendix A

In a porous material, mean intercept length, *MIL*, is the average of the mean solid chord length, *MSC*, and the mean pore chord length, *MPC*.

$$MIL = \frac{(MSC + MSC)}{2} \qquad (A1)$$

Lineal fraction of solid, L_L, is

$$L_L = \frac{MSC}{(MSC + MPC)} \qquad (A2)$$

so

$$MPC = (1 - L_L)2MIL \qquad (A3)$$

If these measurements are averaged over the entire test area, average L_L is equal to A_A [1–3]. The above equation becomes

$$MPC = (1 - A_A)2MIL \qquad (A4)$$

MPC can be related to the average pore dimensions, a and b, by assuming that *MPC* represents the average of uniformly distributed chord lengths across an ellipse of average pore dimensions. If the principal radius, a, corresponds with the 1-direction, MPC_1 can be found by averaging chord lengths in the 1-direction over the diameter in the 2-direction, $2b$. The integral of all chord lengths in a given direction is the area of the ellipse. MPC_1 will be

$$MPC_1 = \frac{\pi ab}{2b} = \frac{\pi a}{2} \qquad (A5)$$

Likewise,

$$MPC_2 = \frac{\pi b}{2} \qquad (A6)$$

Therefore, by combining Equations A4, A5 and A6:

$$a, b = \frac{4}{\pi}(1 - A_A)MIL_1, MIL_2 \qquad (A7)$$

Appendix B

In porous materials mean intercept length, *MIL*, is related to mean pore chord length, *MPC*, by

$$MPC = (1 - A_A)2MIL \qquad (B1)$$

(derived in Appendix A). If mean intercept length measurements are averaged over the entire test volume, average A_A equals V_V [1–3].

$$MPC = (1 - V_V)2MIL \qquad (B2)$$

It is very difficult to average these measurements over the entire test volume without destroying the specimen. Therefore measurements made on six faces of a cubic specimen are assumed to represent the average properties of the specimen. *MPC* can be related to the radii of an ellipsoid that has average pore dimensions by averaging pore chord lengths in one direction within an ellipsoid. If the 1-direction corresponds to the principal radius a, of the ellipsoid, MPC_1 can be found by integrating all chord lengths in the 1-direction and dividing by the cross-sectional area transverse to the 1-direction. The integral of all chord lengths in a given direction within an ellipsoid is the volume of the ellipsoid.

Therefore, MPC_1 is

$$MPC_1 = \frac{(4\pi/3)abc}{(\pi bc)} = 4a/3 \qquad (B3)$$

By combining Equations B2 and B3

$$a = \tfrac{3}{2}(1 - V_V)MIL_1 \qquad (B4)$$

Similarly, b and c are

$$b = \tfrac{3}{2}(1 - V_V)MIL_2 \qquad (B5)$$

$$c = \tfrac{3}{2}(1 - V_V)MIL_3 \qquad (B6)$$

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