RELATIONSHIP BETWEEN SPECIFIC SURFACE AREA AND SPATIAL CORRELATION FUNCTIONS FOR ANISOTROPIC POROUS MEDIA

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ABSTRACT

A result of Debye, Anderson, and Brumberger for isotropic porous media states that the derivative of the two-point spatial correlation at the origin is equal to minus one-quarter of the specific surface area. This result is generalized for non-isotropic media by noting that the angular average of the anisotropic two-point spatial correlation function has the same relationship to the specific surface area.

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I. INTRODUCTION

Debye, Anderson, and Brumberger[1] have shown that, for isotropic porous media, the derivative of the two-point spatial correlation at the origin is equal to minus one-quarter of the specific surface area. The two-point correlation function can be obtained from pictures of cross-sections of a material using image processing techniques.[2] Then, the specific surface area can be measured using the result of Debye et al.[1] The practical importance of this result has been demonstrated recently by combining the measured values of specific surface area with a Kozeny-Carman relation to obtain estimates of fluid permeability.[3]

Since we do not always know that the porous material to be analyzed is isotropic, an important question arises concerning the applicability of the result of Debye et al. for possibly non-isotropic media. We generalize their result to anisotropic media by noting that the angular average of the any two-point spatial correlation function has the same relationship to the specific surface area. Thus, if the two-point correlation function is computed from images by taking angular averages (as has typically been proposed[2]), the slope at the origin will provide a valid estimate of the specific surface area regardless of the degree of anisotropy of the sample.

II. ANISOTROPIC POROUS MEDIA

For a porous material, we define a characteristic function $f(\vec{x}) = 0$ or 1. Then, we say that void regions have $f = 1$, while material regions have $f = 0$. The first two void-void correlation functions are then given by

$$\hat{S}_1 = < f(\vec{x}) > = \phi, \tag{1}$$

and

$$\hat{S}_2(\vec{r}_1, \vec{r}_2) = < f(\vec{x} + \vec{r}_1) f(\vec{x} + \vec{r}_2) > . \tag{2}$$

The brackets $< \cdot >$ indicate a volume average over the spatial coordinate $\vec{x}$. The void volume fraction (or porosity) is given by ϕ. We refer to these two correlation functions as the one- and two-point correlation functions, respectively. For isotropic materials, the one- and two-point correlations can in principle be measured by processing representative images of material cross sections. However, for anisotropic materials, multiple images in orthogonal planes are required to obtain all the necessary information. In general, we still assume that the porous medium of interest is statistically homogeneous so that on average only the differences in the coordinate values are significant (translational invariance). With these assumptions, the two-point correlation function simplifies to

$$\hat{S}_2(\vec{r}_1, \vec{r}_2) = S_2(\vec{r}_2 - \vec{r}_1). \tag{3}$$

From Eq. (2), it follows that

$$S_2(\vec{r}) = \frac{1}{V} \int_V d^3x f(\vec{x}) f(\vec{x} + \vec{r}), \tag{4}$$

where V is total volume of integration. Two important facts about the two-point correlations for applications to random media are

$$S_2(0) = \phi \tag{5}$$

and

$$\lim_{|\vec{r}| \to \infty} S_2(\vec{r}) = \phi^2. \tag{6}$$

The theorem that we wish to prove states that

$$A_2'(0) = -s/4, \tag{7}$$

where s is the specific surface area (internal surface area per unit volume) and the angular average of $S_2(\vec{r})$ is defined by

$$A_2(r) = \frac{1}{4\pi} \int d\varphi d\theta sin\,\theta S_2(r\hat{r}) = \frac{1}{4\pi V} \int d\varphi d\theta sin\,\theta \int_V d^3x f(\vec{x}) f(\vec{x} + r\hat{r}), \tag{8}$$

where $\hat{r} = \hat{r}(\theta, \varphi)$ is the radial unit vector.

The derivation of Eq. (7) proceeds as follows: Taking the derivative of Eq. (8) gives

$$\frac{dA_2(r)}{dr} = \frac{1}{4\pi V} \int d\varphi d\theta sin\,\theta \int_V d^3x f(\vec{x}) \frac{\partial f(\vec{x} + r\hat{r})}{\partial r}. \tag{9}$$

Defining the pore volume as V_p, we have

$$\frac{dA_2(r)}{dr} = \frac{1}{4\pi V} \int d\varphi d\theta sin\,\theta \hat{r} \cdot \int_{V_p} d^3x \nabla f(\vec{x} + r\hat{r}). \tag{10}$$

Then, if da_s is an infinitesimal element of the material surface area a_s, we have

$$\frac{dA_2(r)}{dr} = \frac{1}{4\pi V} \int_{a_s} da_s \int d\varphi d\theta sin\,\theta \hat{r} \cdot \hat{n}_s f(\vec{x}_s + r\hat{r}), \tag{11}$$

where $\hat{n}$ is the unit outward normal vector at the surface position given by $\vec{x}_s$. Now, if we let $r \to 0^+$ and center the coordinate system at $\vec{x}_s$ with $\hat{n} = \hat{z}$, we find that

$$\int d\varphi d\theta sin\,\theta \hat{r}\cdot\hat{n}_s f(\vec{x}_s + 0^+\hat{r}) = 2\pi \int d\theta sin\,\theta cos\,\theta f(\vec{x}_s + 0^+\hat{r}) = 2\pi \int_{-1}^{0} d\mu\mu = -\pi \qquad (12)$$

and we obtain a definite result for Eq. (11) given by

$$\lim_{r\to 0^+} \frac{dA_2(r)}{dr} = -\frac{a_s}{4V}. \qquad (13)$$

Since the specific surface area is defined as $s = a_s/V$, Eq. (13) is equivalent to Eq. (7). Debye et al.[1] used a more intuitive approach to obtain their result for isotropic media.

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REFERENCES

1. P. Debye, H. R. Anderson, Jr., and H. Brumberger, *J. Appl. Phys.* **28**, 679 (1957).
2. J. G. Berryman, *J. Appl. Phys.* **57**, 2374 (1985).
3. J. G. Berryman and S. C. Blair, *J. Appl. Phys.* **60**, 1930 (1986),