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Continuum percolation thresholds for mixtures of spheres of different sizes

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Abstract

Using Monte-Carlo simulations, we find the continuum percolation threshold of a three-dimensional mixture of spheres of two different sizes. We fix the value of r, the ratio of the volume of the smaller sphere to the volume of the larger sphere, and determine the percolation threshold for various values of x, the ratio of the number of larger objects to the number of total objects. The critical volume fraction increases from $\phi_c = 0.28955 \pm 0.00007$ for equal-sized spheres to a maximum of $\phi_c^{\max} = 0.29731 \pm 0.00007$ for $x \approx 0.11$, an increase of 2.7%.

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1. Introduction

Many static and dynamic physical properties of a system are determined by the spatial distribution of the system's components, especially when the system is near a critical point and is beginning to undergo a structural phase transition. Examples of such systems include porous media, composite materials, colloids, polymers, and the distribution of galaxies [1,2].

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Many of these real-world systems are best modeled by continuum percolation in which objects of a given shape and size are randomly distributed, as opposed to site or bond percolation in which sites or bonds in a discrete lattice are randomly occupied. While certain quantities (e.g., the critical exponents) are independent of the details of the percolation model, other quantities such as the percolation threshold are not [2–5].

In previous research ([6–16]) simulations were performed to find the continuum percolation threshold for systems composed of objects of a given shape: spheres, ellipsoids, sticks, and cubes. In this paper, we determine the percolation threshold of a mixture of spheres A and B of two different sizes, v_A and v_B in 3D. We demonstrate that the continuum percolation threshold is dependent on the relative concentrations of the two different sized spheres.

2. Density parameters and scaling function in continuum percolation

Continuum percolation has been characterized by certain parameters [8]:

(i) the density

$$\rho \equiv \frac{N}{V} , \tag{1}$$

where N is the total number of objects and V the volume of the system;

(ii) the dimensionless density

$$\eta = \frac{Nv}{V} = \rho v , \tag{2}$$

where v is the volume of the object; and

(iii) the volume fraction

$$\phi \equiv 1 - \mathrm{e}^{-\eta} . \tag{3}$$

The probability of generating a cluster of size s or greater at a specified η is [1,2]

$$P(s|\eta) \sim As^{2-\tau} f[(\eta - \eta_c)s^{\sigma}] , \tag{4}$$

where both τ and σ are universal exponents and A is a non-universal constant. In 3D the values of τ and σ are 2.18906±0.00006 and 0.4522±0.0008, respectively [17]. Near the percolation threshold the scaling function $f(x)$ can be expanded in a Taylor series

$$f(x) = 1 + Bx + \mathcal{O}(x^2) . \tag{5}$$

Combining Eqs. (4) and (5)

$$P(s|\eta)s^{\tau-2} \sim A + AB(\eta - \eta_c)s^{\sigma} + \cdots . \tag{6}$$

Thus, $P(s|\eta)s^{\tau-2}$ becomes constant at the percolation threshold as s becomes asymptotically large.

For systems composed of N_A objects of volume v_A, and N_B objects of volume v_B, the percolation threshold is a function of the relative concentration of the objects and the ratio

$$r \equiv \frac{v_B}{v_A} . \tag{7}$$

Eq. (2) can be generalized as

$$\eta \equiv \frac{N_A v_A}{V} + \frac{N_B v_B}{V} \equiv \eta_A + \eta_B = \rho[x(v_A - v_B) + v_B]$$
$$= \rho v_A[x(1-r) + r]$$
$$= \eta(x, r) , \quad (8)$$

where $x \equiv N_A/N$, and $N = N_A + N_B$ is the total number of the objects in the simulation. Eq. (3) is generalized to

$$\phi = 1 - e^{-(\eta_A + \eta_B)} = 1 - e^{-\eta} , \quad (9)$$

as shown in the appendix.

3. Simulation and methods

We use Monte-Carlo simulations to find the continuum percolation threshold for a mixture of two different sized spheres. Recently, simulations using gradient percolation for soft discs of two different radii were performed in 2D [12], unfortunately this method cannot be applied in three dimensions. The method used here is the same as that used in previous work [15], and is based on the Leath algorithm [18] and the Lorenz and Ziff method [8], which use Fisher's ansatz scaling function (Eq. (4)).

We determine the location of an object randomly using an uniform distribution. We determine whether an object is of size v_A or v_B as follows. We generate random number between 0 and 1. If the number is less than the relative concentration x chosen for the simulation, the object is of type A, otherwise it is of type B.

In order to optimize the calculations, the edge lengths of the simulation, L, varied from $81 \times 81 \times 81$ for simulations dominated by small objects to $141 \times 141 \times 141$ for simulations dominated by large objects.

We tested our simulation methods by reproducing the 2D results of Ref. [12] for interpenetrating discs of radius 1.0 and 0.5 at $x = 0.30$ for a system of size $L = 201$. We found $\phi = 0.6881 \pm 0.0001$ (Fig. 1), consistent with the value found previously [12].

4. Results

For a binary distribution of spheres, the volume fraction (9) can be written as

$$\phi(x, \lambda) = 1 - e^{-\langle n \rangle (\pi/6)[x(1-\lambda^3)+\lambda^3]} , \quad (10)$$

where $\lambda \equiv r^{1/3}$ is the ratio of the two radii of spheres and $\langle n \rangle$ the mean number of spheres per unit volume.

The percolation threshold results in this work are for fixed $\lambda = 0.5$. The volume of the bigger sphere is eight times greater than that of the smaller sphere. In Fig. 2 we illustrate the method for determining ϕ_c for the relative concentration $x = 0.25$ and

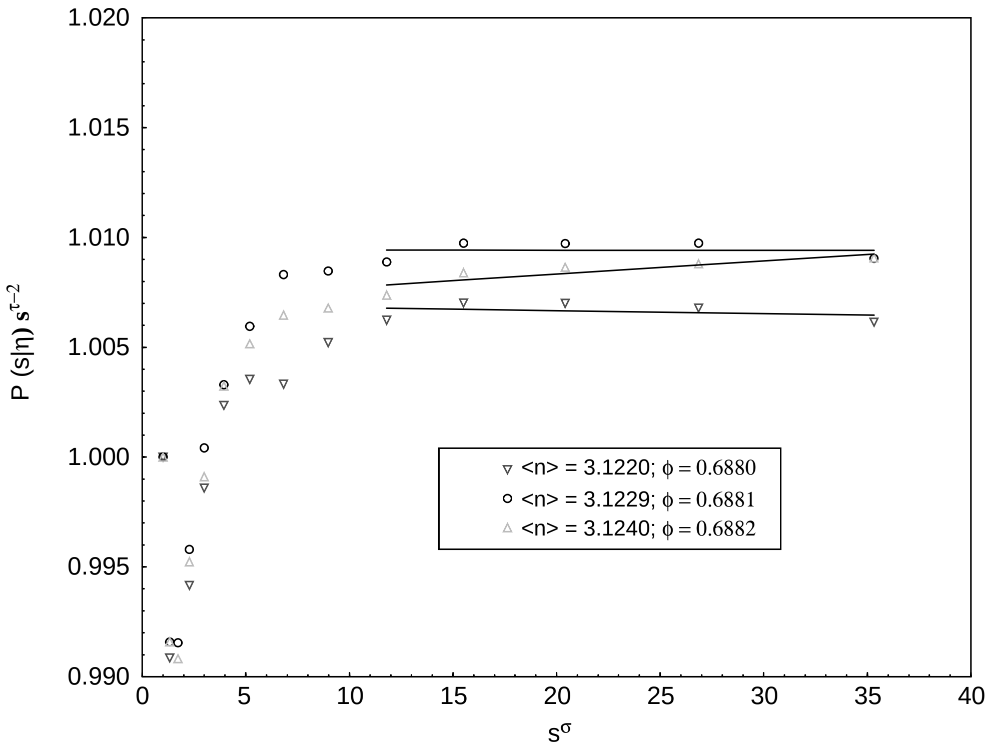

Fig. 1. $\phi_c(x, \lambda)$ for two different sized discs for relative concentration $x = 0.30$ and ratio of the two radii $\lambda = 0.5$. In the simulation, 100,000 realizations are performed in a 201 × 201 square grid with cell edge equal to the diameter of the larger disc. The estimated threshold is $\phi_c(0.3, 0.5) = 0.6881 \pm 0.0001$.

estimate

$$\phi_c(x = 0.25; \lambda = 0.5) = 0.29537 \pm 0.00007 . \qquad (11)$$

Percolation thresholds are shown in Table 1 for $x=0$, 0.10, 0.11, 0.15, 0.25, 0.50, 0.75, and 1.0. In Fig. 3 we plot ϕ_c as a function of x at fixed volume ratio $r=\lambda^3=0.125$. The fitted curve has qualitatively the same form as that obtained for discs. The concentration value $x = 0.11$ corresponds approximately to the maximum percolation threshold for $\lambda = 0.5$. That is,

$$\phi_c^{\max} = 0.29731 \pm 0.00007 . \qquad (12)$$

Here $\phi_c^{\max}$ is 2.69% larger than the ϕ_c for objects of equal size for which $\phi_c(x=0)=\phi_c(x=1)=0.28955 \pm 0.00007$.

5. Discussion and conclusions

The main focus of this work is to determine the dependence of the percolation threshold for systems of two different sized spheres. The results show that the percolation threshold is dependent on the relative concentration of the spheres. This is similar to the behavior of discs in 2D [12] and in contrast to the work of Ref. [19] in which it

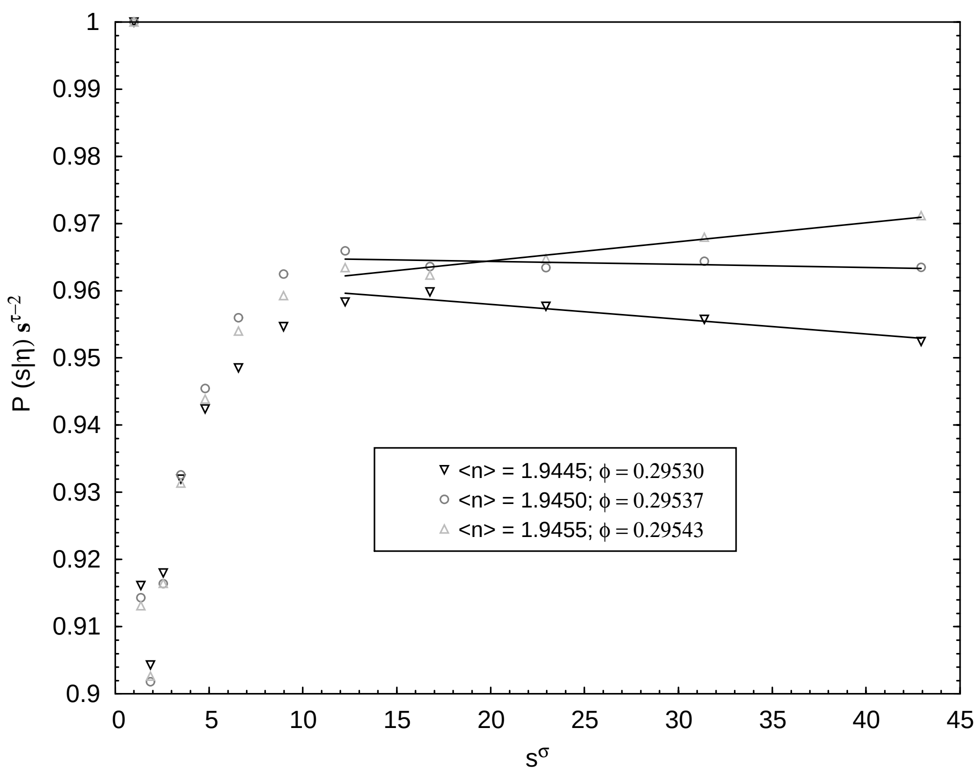

Fig. 2. Estimate of the percolation threshold $\phi_c(x,\lambda)$ for spheres with relative concentration $x = 0.25$ and ratio of the two radii $\lambda = 0.5$. In the simulation, 100,000 realizations are performed in a $81 \times 81 \times 81$ cubic grid with cell edge equal to the diameter of the larger sphere. The measured threshold is $\phi_c(0.25, 0.5) = 0.29537 \pm 0.00007$.

Table 1
Values of the percolation threshold $\phi_c(x, \lambda = 0.5)$ for soft core spheres for various values of relative concentration x

x	0	0.10	0.11	0.15	0.25	0.50	0.75	1.0
ϕ_c	0.28955	0.29730	0.29731	0.29700	0.29537	0.29233	0.29065	0.28955

The values have an estimated error $\pm 7 \times 10^{-5}$.

was not possible to discern a dependence of ϕ_c on relative concentration for cubes of two different sizes. Our results are also consistent with the results for void percolation in 3D in which a dependence of ϕ_c on relative concentration is found [4].

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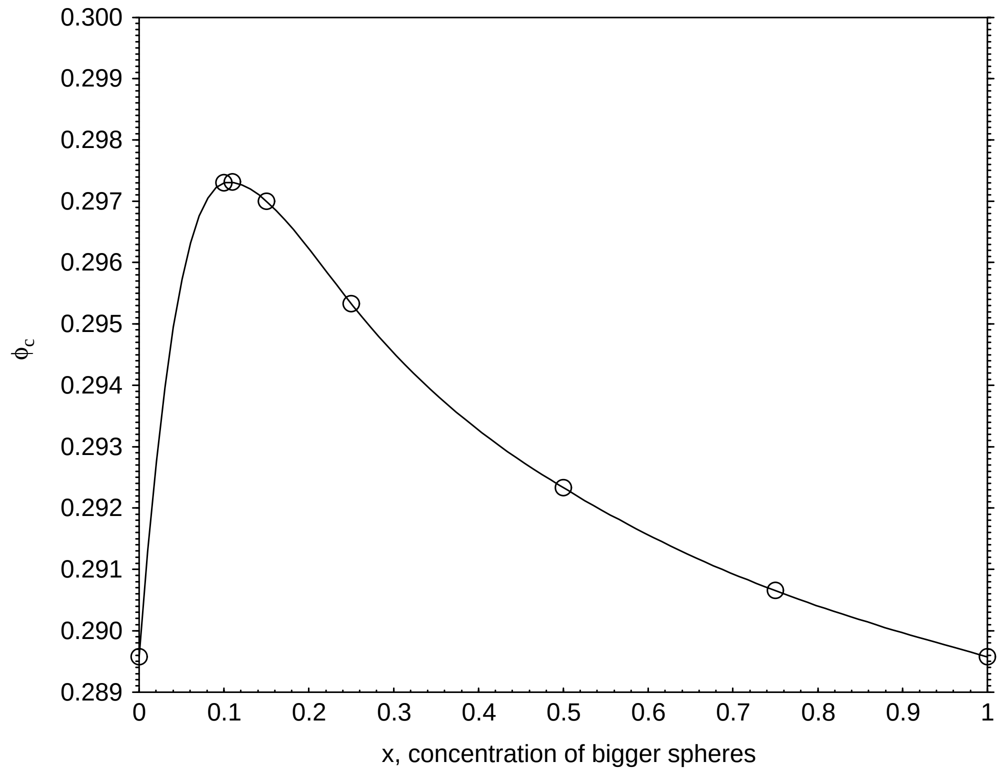

Fig. 3. Percolation threshold $\phi_c(x,\lambda)$ versus x mixtures of different sized spheres. The line is a fitted spline. The values have an estimated error $\pm 7\times 10^{-5}$. The critical volume of ϕ_c for $x=0$ and 1 corresponding to equisized spheres is $\phi_c = 0.28955$.

Appendix A. Volume fraction equation

The volume fraction for soft core objects of a single size in continuum percolation is given by Eq. (3). Following Ref. [20], this equation is extended here to systems containing soft core objects of multiple sizes. Since the probability that a point in volume V is contained within one object of size v is v/V, and this probability is independent of the probability of the point being contained within any other objects, it is possible to write the probability Q that a point in a volume V is not contained within any of the N_A objects of volume v_A, N_B objects of volume v_B, etc.,

$$Q = \left[1-\left(\frac{v_A}{V}\right)\right]^{N_A}\left[1-\left(\frac{v_B}{V}\right)\right]^{N_B}\cdots$$
$$= \left[1-\left(\frac{\eta_A}{N_A}\right)\right]^{N_A}\left[1-\left(\frac{\eta_B}{N_B}\right)\right]^{N_B}\cdots\,. \quad (A.1)$$

In the limit $V, N_A, N_B, \ldots \to \infty$, where η_A, η_B are constant, (A.1) yields

$$Q = \mathrm{e}^{-(\eta_A+\eta_B+\cdots)}\,. \quad (A.2)$$

Finally, we obtain the generalization of (3) for systems containing objects of different sizes

$$\phi = 1 - Q = 1 - e^{-(\eta_A + \eta_B + \cdots)} \equiv 1 - e^{-\eta} \,. \tag{A.3}$$

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