

INFLUENCE OF SCATTERER'S GEOMETRY ON POWER-LAW FORMULA IN RANDOM MIXING COMPOSITES

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Abstract—To apply the power-law to random mixing composites, the power parameter α is defined as the mean depolarization factor along the external field. The formula of α is derived from the effective medium theory and beta function distribution assumption to study the geometrical influence of scatterers. According to the simulation, we prove that $\alpha = 1/3$ is fit to the composites of randomly distributed spherical dielectric scatterers, whereas $\alpha = 1/2$ to the flake-like or cylindrical shaped scatterers. This law can be applied to both dilute and dense condition describing the effective permittivity of random mixing composites and extended to aligned cases, which are meaningful to practical applications.

1. INTRODUCTION

Various mixing models have been developed to solve the effective dielectric parameters of composites since the mid-1800 [1]. These models, such as the Maxwell Garnett rule, Bruggeman's formula, and other mixing rules based on effective medium theory, are still

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widely used and are attracting much interest in new applications [2–7]. However, the Maxwell Garnett rule and other rules derived from this origin are not suitable for dense materials [8]. In practical random medium theory and applications requiring a wide density choice, a large set of mixing rules have been introduced by writing the ‘power-law’ approximation:

$$\varepsilon_{eff}^{\alpha} = \sum_{i=1}^N f_i \varepsilon_i^{\alpha} \quad (1)$$

with ε_{eff} , f_i , and ε_i as the effective relative permittivity of the composites, volume fraction, and relative permittivity of the i th phase. These formulas, first suggested by Lichtenecker [9], have been used by many authors for different situations with certain value of α . For example, in the Birchak formula [10] the parameter α is 1/2, which have been existing for a long time in the field of optical physics to deal with refractive index measurement. The linear law [11], which corresponds to $\alpha = 1$ in Eq. (1), can be given theoretical explanation if the mixture is formed of plates or other inclusions without induced depolarization. Jacobsen and Schjonning [12] found that the parameter α can vary from 0.4 to 0.8, based on experimental data from moist mineral soils. The different background and a lack of universal theoretical support resulted in power-law being generally considered as only an empirical tool for a long time.

In 1999, Zakri et al. [13], established a theoretical model for this mixing formula using the effective medium theory together with the assumption of self-consistency. A beta function distribution of the geometrical shapes of inclusions is also introduced. However, the physical meaning of parameter α is still unclear. Recently, the power-law used to describe a fracture size distribution has been studied for the percolation effect of porous effective medium, and the authors also set up the expression of effective parameter in a complex function [14, 15]. If we can attribute the geometrical effect into the parameter α rather than the power-law formula, a simple form to express the effective parameter will be achieved and it will be more favorable for different applications. Therefore, the purpose of this work is to explore the application of simple power-law to complex dielectric mixture by identifying the meaning of α based on Tarik Zakri’s method. Composites of inclusions as sub-wavelength sized spherical, flake-like, and cylindrical scatterers with dispersive permittivity will be simulated for comparison in a wide range of volume fraction.

2. THEORETICAL METHOD

According to the effective medium theory [16], two approaches can be used to evaluate the effective permittivity:

- (i) a discrete approach whereby the medium is considered as a network of resistances or capacitances and
- (ii) a continuous approach whereby each phase is constituted from particles included in a host medium.

We use the latter approach. The effective relative permittivity of composite of N phases yields

$$\sum_{i=1}^N f_i \left(1 - \frac{\varepsilon_i}{\varepsilon_{eff}} \right) C_i = 0 \quad (2)$$

by introducing the field ratio $C_i = \bar{E}_i / \bar{E}_0$ between the local electrical field in the i th phase and the uniform field. If we consider now the case of an ellipsoidal scatterer of permittivity ε_i in a homogeneous medium of permittivity ε_m as shown in Fig. 1, and placed it in a uniform electrical field E_0 , the corresponding C_i factor can be expressed by [17]

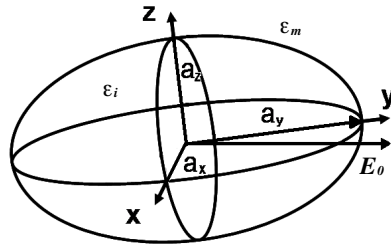


Figure 1. A dielectric ellipsoidal inclusion of permittivity ε_i in a matrix of permittivity ε_m under an external field E_0 .

$$C_i = \sum_{j=1}^3 \frac{\cos^2 \varphi_{ij}}{1 + N_{ij} \left(\frac{\varepsilon_i}{\varepsilon_{eff}} - 1 \right)} \quad (3)$$

where φ_{ij} are the space angles between the three main axes x ($j = 1$), y ($j = 2$), and z ($j = 3$) of the ellipsoid of the i th phase and the direction of external field E_0 , and N_{ij} are the depolarization factors. For an ellipsoid, N_{ij} are expressed by Landau and Lifschitz [18] as,

$$N_{ij} = \frac{a_1 a_2 a_3}{2} \int_0^\infty \frac{du}{(u + a_j)(u + a_1)^{1/2}(u + a_2)^{1/2}(u + a_3)^{1/2}} \quad (4)$$

where a_j denote the semi-axes of the ellipsoid in the three directions. The space angles are constrained such that

$$\sum_{j=1}^3 \cos^2 \varphi_{ij} = 1. \quad (5)$$

According to Tarik Zakri's method [13], the scatterers' shapes are not considered to be uniform but follow a beta function distribution. Therefore, equivalent depolarization factor of phase i in the direction of the external electrical field, N_{iE} , is introduced as a variable of the probability density function [19] of the beta function distribution in the following form:

$$P_\alpha(N_{iE}) = \frac{\Gamma(2)}{\Gamma(1-\alpha)\Gamma(1+\alpha)} N_{iE}^{-\alpha} (1-N_{iE})^\alpha \quad (6)$$

where Γ is the gamma function, and $0 \leq N_{iE} \leq 1$. The component with space angle in Eq. (3), which describes the influence of scatterer's space distribution, can be rewritten with concern over the beta function distribution. Consequently, the C_i factors can be transformed from Eq. (3) to

$$C_i = \int_0^1 \frac{P_\alpha(N_{iE})}{1 + N_{iE} \left(\frac{\varepsilon_i}{\varepsilon_{eff}} - 1 \right)} dN_{iE}. \quad (7)$$

Substituting Eq. (7) into Eq. (2), we get Eq. (1) after some mathematical derivation [13]. Therefore, it is proved that power-law formulae are physically sound.

Our aim is to explore the physical meaning of factor α and its formula based on the above analysis. According to the characterization of $P_\alpha(N_{iE})$ function [19], α is related to the mean value of variable N_{iE} which can be solved by effective medium method. In effective medium, the averaging relations interconnect the field terms and dipole moments within scatterers. The components of local field of phase i along the main axes are given as,

$$E_{ij} = E_0 \cos \varphi_{ij} + \frac{N_{ij}}{\varepsilon_{eff}} P_{ij} \quad (8)$$

where P_{ij} are the polarization density along the axes featuring the local dipole moments. Since P_{ij} are dependent on the applied field, we can write,

$$P_{ij} = np_i E_0 \cos \varphi_{ij} \quad (9)$$

with p_i the polarizability of phase i . Then by transforming the components back to E_0 direction and using Eq. (5), the expression of local field along the direction of E_0 is rewritten as

$$E_{iE} = \sum_{j=1}^3 E_{ij} \cos \varphi_{ij} = E_0 + \frac{np_i E_0}{\varepsilon_{eff}} \sum_{j=1}^3 N_{ij} \cos^2 \varphi_{ij}. \quad (10)$$

To find N_{iE} , we write Eq. (10) in a similar form like Eq. (8). The polarization density along the direction of E_0 is $P_{iE} = np_i E_0$. Therefore, the summation part of Eq. (10) should be attributed to N_{iE} . Accordingly,

$$N_{iE} = \sum_{j=1,2,3} N_{ij} \cos^2 \varphi_{ij} \quad (11)$$

and Eq. (10) becomes

$$E_{iE} = E_0 + \frac{N_{iE}}{\varepsilon_{eff}} P_{iE}. \quad (12)$$

The same form as Eq. (8) but in the direction of external field.

Since α is the shape factor in Eq. (6), of relevance to mean variable as discussed before, here we define it as the mean value of N_{iE} . In the case of random distribution and suppose that all the phases has the same geometrical features, says N_{ij} , we have

$$\alpha = \langle N_{iE} \rangle = \sum_{j=1}^3 \frac{2}{\pi} \int_0^{\frac{\pi}{2}} N_{ij} \cos^2 \varphi_{ij} d\varphi_{ij}. \quad (13)$$

With this approach, the influences of scatterer's geometry and distribution are introduced to the power parameter in power-law formula with respect to the depolarization factors and the spacing angles. If the phases of the composite have different geometrical features, Eq. (13) changes to a summation of mean N_{iE} multiplied by the volume ratio of phase i to all the phases except the host medium, because the host medium is considered as a shapeless component during the derivation. In next two sections, several common cases will be discussed to verify this definition and illustrate its application.

3. CASE STUDIES

By virtue of the simple form and predictable power parameter, power-law is favorable for practical uses. In the two-phase model to be studied, dielectric scatterers with three generic configurations,

spherical, flake-like, and cylindrical shape, are random distributed in the host dielectric medium respectively and studied using the power-law formula, finite-different time-domain (FDTD) method, and other effective medium approximations. As shown in Fig. 2, spherical, flake-like, and cylindrical scatterers are located in the host medium with both random orientation and position. The relative permittivity and permeability of host medium are $\varepsilon_m = 2$, $\mu_m = 2$, and scatterer's parameters are with Debye's dispersion,

$$\varepsilon_i = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 - i\omega\tau}, \text{ and } \mu_i = \mu_\infty + \frac{\mu_s - \mu_\infty}{1 - i\omega\tau} \quad (14)$$

where parameters $\varepsilon_s = 20$, $\mu_s = 20$, $\varepsilon_\infty = 1$, $\mu_\infty = 1$, and $\tau = 6 \times 10^{-11}$ s. The sizes of scatterers (the largest dimensions) are 2 mm, much smaller than the wavelength in the simulating frequency range 1–15 GHz.

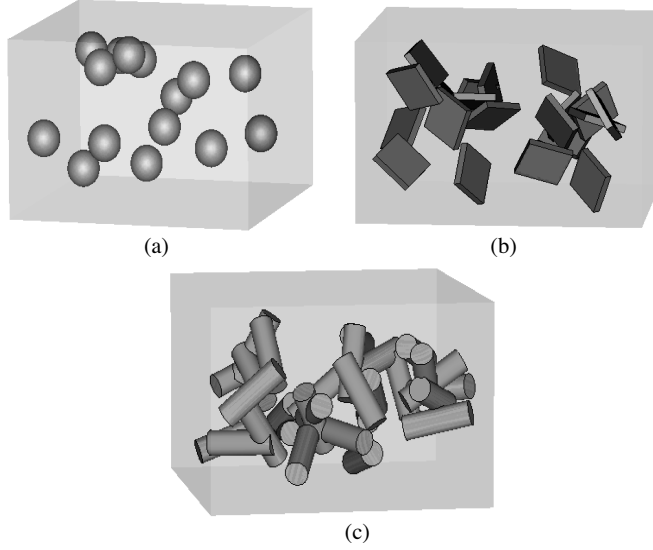


Figure 2. Diagrams of the two-phase composite filled with (a) spherical scatterers, (b) flake-like scatterers, and (c) cylindrical scatterers.

3.1. Power-law Method

For spherical scatterers, the depolarization factors remain 1/3 along any arbitrary directions. Therefore, suppose the applied field is along one of the feature axis x , the space angles for the other two axes should

be $\pi/2$, then Eq. (13) reduces to contain only x component,

$$\alpha_{sphere} = \langle N_{iE} \rangle = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \frac{1}{3} \cos^2 \theta d\theta = \frac{1}{3}.$$

For flake-like scatterers, if the width is tens of times the thickness, in-plane depolarization factors can be considered to be zero ($N_x = N_y$) and the out-of-plane depolarization factor is 1 ($N_z = 1$). As a consequence, only one component is considered,

$$\alpha_{flake} = \langle N_{iE} \rangle = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} 1 \cos^2 \theta d\theta = \frac{1}{2}.$$

In the case of cylindrical scatterers, when the height is tens of times the diameter, the depolarization factor in the axial direction is almost zero ($N_z = 0$) and the radial ones are 1/2 ($N_x = N_y$). As a result, Eq. (13) has two equal components,

$$\alpha_{cylinder} = \langle N_{iE} \rangle = 2 \times \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \frac{1}{2} \cos^2 \theta d\theta = \frac{1}{2}.$$

Then, the effective permittivity of composites with scatterers of different shape is calculated using Eq. (1). Before this work, power-law with α 's value at 1/3 and 1/2 can be found in literatures [9, 20, 21] but applied in different backgrounds, therefore it is difficult to figure out the physical meaning of α . In this paper, power-law is applied to scatterers with same composition under the same background but with different geometrical features.

3.2. FDTD Method

Commercial software CST Microwave Studio® is used to model the reflecting and transmitting parameters of the composites discussed above. With a high fractional volume, scatterers may intersect with each other. All models are implemented with the same set of accuracy (−60 dB) and mesh scale. To achieve the correct simulation results in random distribution cases, each case has been modeled more than 15 times, which means rebuilding the structure and averaging the output data, and each model repeatedly simulated times to confirm the stable result. Therefore, we are promising to get credible results. Based on the scattering parameters, the effective permittivity is retrieved using the retrieving method introduced in [22].

3.3. Other Effective Medium Methods

The Maxwell Garnett rule (MG) and Bruggeman's formula (BF) are applied to the cases to predict the effective permittivity of composites, comparing with the power-law method. The Maxwell Garnett rule for random distributing mixture (two phases) is given as [16],

$$\varepsilon_{eff_MG} = \varepsilon_m + \varepsilon_m \frac{\frac{f_i}{3} \sum_{j=1}^3 \frac{\varepsilon_i - \varepsilon_m}{\varepsilon_m + N_{ij}(\varepsilon_i - \varepsilon_m)}}{1 - \frac{f_i}{3} \sum_{j=1}^3 \frac{\varepsilon_i - \varepsilon_m}{\varepsilon_m + N_{ij}(\varepsilon_i - \varepsilon_m)}}. \quad (15)$$

Bruggeman's formula for the same situation is,

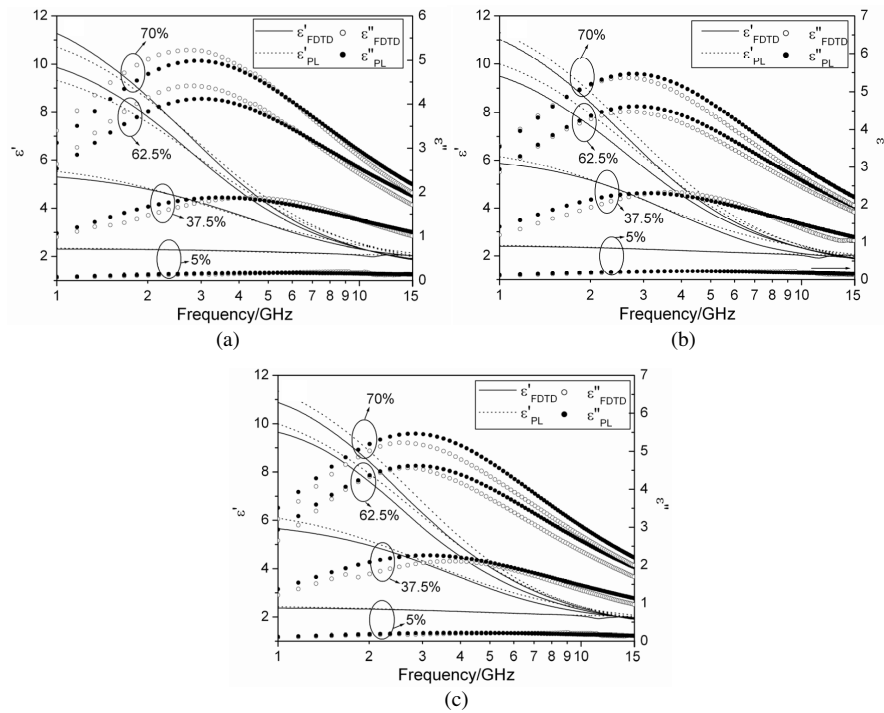


Figure 3. Effective permittivity of the composite of (a) spherical, (b) flake-like, and (c) cylindrical scatterers with variant volume fraction as a function of frequency. The subscript FDTD means the data from FDTD simulation, and PL means the result of power-law method.

$$\epsilon_{eff_BF} = \epsilon_m + \epsilon_a \frac{\frac{f_i}{3} \sum_{j=1}^3 \frac{\epsilon_i - \epsilon_m}{\epsilon_a + N_{ij}(\epsilon_i - \epsilon_m)}}{1 - \frac{f_i}{3} \sum_{j=1}^3 \frac{\epsilon_i - \epsilon_m}{\epsilon_a + N_{ij}(\epsilon_i - \epsilon_m)}} \quad (16)$$

where $\epsilon_a = \epsilon_{eff} - N_{ij}(\epsilon_{eff} - \epsilon_m)$ [16].

4. RESULTS AND DISCUSSION

As shown in Fig. 3, the effective permittivity calculated by FDTD and power-law method for the spherical, flake-like, and cylindrical scatterers' cases are close to each other in both a wide volume fraction range and frequency range. To make a better understanding of

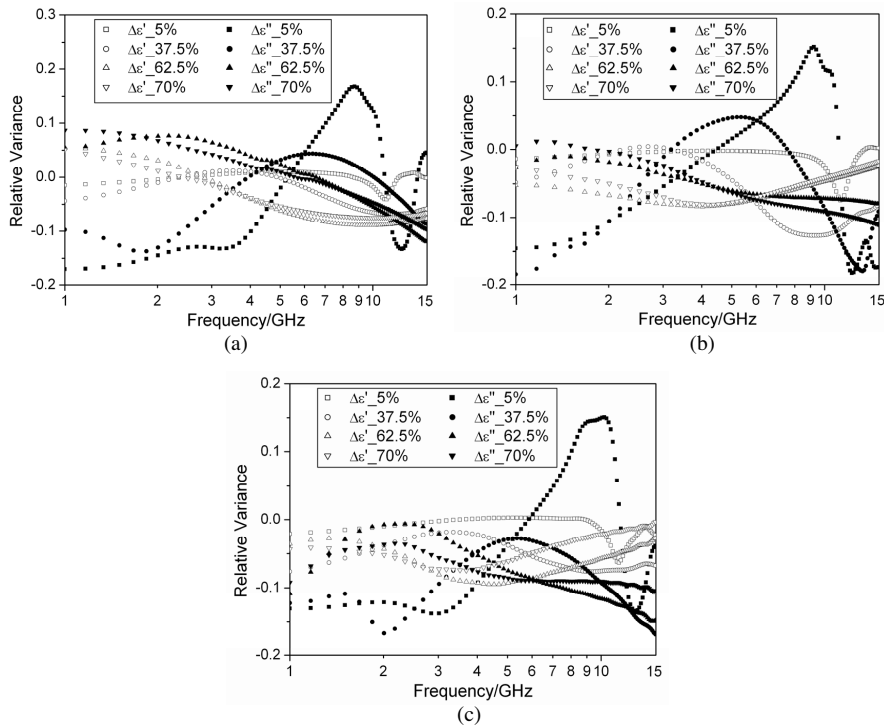


Figure 4. Relative variance of the effective permittivity from Fig. 1 for the composites of (a) spherical, (b) flake-like, and (c) cylindrical scatterers as a function of frequency.

deviation, relative variance of the real and imaginary part of effective permittivity are calculated by the following formulas and are shown in Fig. 4,

$$\Delta\varepsilon' = \frac{\varepsilon'_{FDTD} - \varepsilon'_{PL}}{\varepsilon'_{FDTD}}, \text{ and } \Delta\varepsilon'' = \frac{\varepsilon''_{FDTD} - \varepsilon''_{PL}}{\varepsilon''_{FDTD}} \quad (17)$$

with subscripts FDTD and PL denoting the FDTD and the power-law method respectively. With a relative variance smaller than 0.2, the above conclusion of general agreement between the two methods holds in a wide volume fraction range from 5% to 70%, dilute to dense cases, and is quite favorable since many effective medium methods experience large deviation in either the dilute or the dense situation.

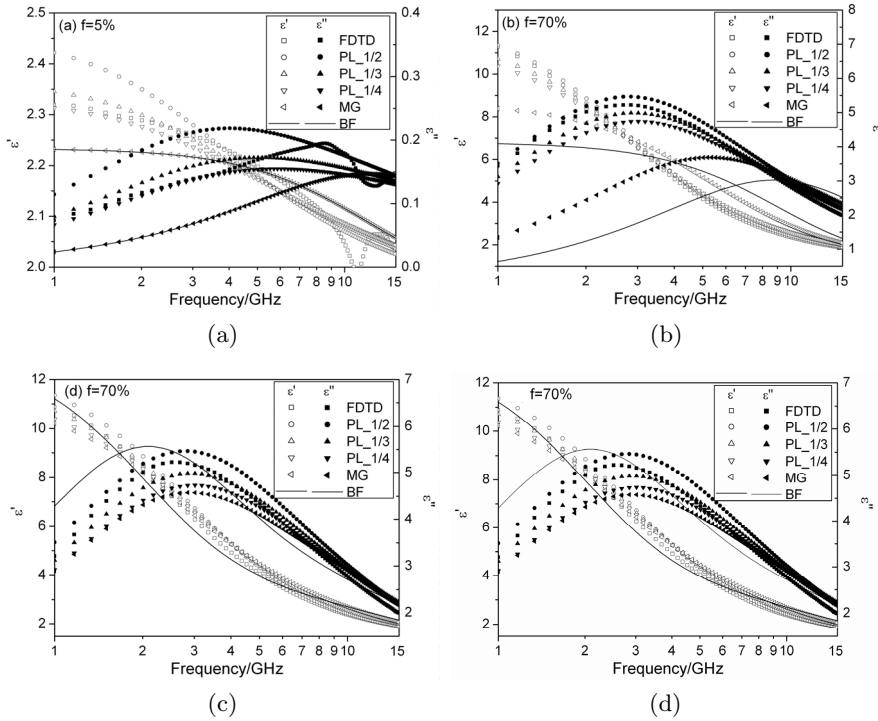


Figure 5. The effective permittivity for the composites of spherical scatterers (a), (b) and cylindrical (c), (d) scatterers at the dilute (5%) and dense (70%) volume fraction. The open symbols denote the real part of the effective permittivity calculated by FDTD method, power-law method with $\alpha=1/2$, $1/3$, and $1/4$, Maxwell Garnett rule (MG) and Bruggman formula (BF), whereas the solid symbols denote the imaginary part of the effective permittivity.

As can be seen in Fig. 4, a relatively extensive deviation is observed in the 5% case for the imaginary part of the effective permittivity. This happens at a frequency where an unexpected resonance is found in the FDTD result as shown in Fig. 3 or Figs. 5(a) and (c). Considering the potential influence of location and orientation in FDTD method, we have simulated the random distribution of scatterers in twenty times and averaged out the results for each case. Therefore, the deviation is not related to inhomogeneous distribution but a kind of dimensional resonance corresponding to the effective size and wave length of the mixture.

Comparisons between FDTD and several effective medium methods for both dilute and dense case are shown in Fig. 5. The power-law series are closest to the FDTD results both in the dilute and dense case. MG and BF method have the same result in dilute case but far from the others in spherical case. However, for the dense cylindrical case, MG and BF have closer predictions. It seems that both MG and BF methods are unstable with respect to scatterer's density and geometry, which has also been suggested in other literatures too [23]. Power-law is more suitable in these cases.

The definition of the α parameter as the mean depolarization factor of the inclusions along the external field direction can be used to explain the existing power-laws. In Fig. 6, the effect of α 's value on the probability function, Eq. (6), is demonstrated. When $\alpha = 0$, the probability function becomes a uniform one, which shows a mean geometrical feature, and Eq. (1) reduces to Lichtenecker's law regardless of inclusion's geometry. When $\alpha = 1$, the function has infinite value at the point where $N_{iE} = 0$, which means that the external field is along the direction where $N_{iE} = 0$, e.g., in the case

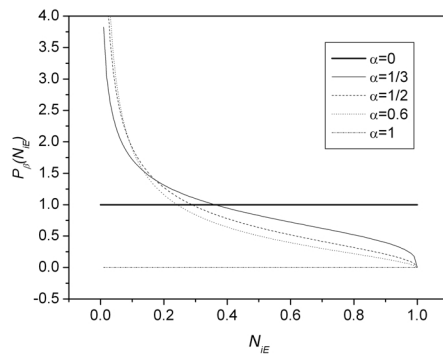


Figure 6. Probability function of beta function distribution of inclusion for various values of α factor.

of porous composite, all the pores should be parallel to the external field, and Eq. (1) reduces to linear law for inclusions without induced depolarization. Overall, limitations of power-law, as well as other effective medium methods, are due to the neglecting of the scatterer's size, interaction, and so on. Therefore, in some specific cases, other complex methods may be more favorable [24, 25], but the simple form and applicability to random mixing material with certain geometrical features in wide volume fraction range are the advantages for power-law.

5. CONCLUSION

In this paper, a method to determine the value of parameter α is suggested by defining it as the mean depolarization factor along the external field. The geometrical influence of scatterers is introduced by this definition. It is demonstrated by FDTD simulation that the power-law formula with $\alpha = 1/3$ is suitable to describe the random distributing spherical scatterers, and $\alpha = 1/2$ to the flake-like and cylindrical cases, in both the dilute and dense condition. With this approach, we enable the simple power-law to predict the effective parameters for composites with random distributing inclusions with specific geometrical feature.

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