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Explicit solutions to the mixing rules with three-component inclusions

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ABSTRACT

The explicit solutions of Bruggeman and Maxwell-Garnett mixing rules with three-component inclusions are provided. For a three-component mixture of aerosol, the comparisons of different methods are shown for refractive index and optical properties.

1. Theory

The optical properties of inhomogeneous composite materials have wide applications in atmospheric science, oceanography, and other fields of geophysical science. For example, the atmospheric aerosol radiative forcing depends on the mixing state of the aerosol. Individual aerosol particles often contain composite (internal) mixtures of different inorganic and organic compounds with very complicated morphology [1,2]. In principle, the existence of numerically exact methods for solving the macroscopic Maxwell equations (e.g., the superposition T-matrix method) are available to calculate the scattering properties of a composed mixture [3–7]. However, these kind of exact methods are very time-consuming and not easy to apply to the study of aerosol radiative forcing in climate models. On the other hand, the effective medium approximation method is traditionally used for dealing with the composite material, and the accuracy of these methods have been analyzed by comparing with the rigorous numerical methods. [2,6,7]. Among the effective medium approximation methods, the Bruggeman mixing rule [8] and Maxwell-Garnett mixing rule [9] are two well-known methods [2,10]. The Bruggeman mixing rule treats all materials on equal base with the mixture of different components attached together. The Bruggeman mixing rule is given by

$$V_1\frac{\epsilon_1-\epsilon}{\epsilon_1+2\epsilon}+V_2\frac{\epsilon_2-\epsilon}{\epsilon_2+2\epsilon}+V_3\frac{\epsilon_3-\epsilon}{\epsilon_3+2\epsilon}+\ldots=0,\quad (V_1+V_2+V_3+\ldots=1), \tag{1}$$

where ϵ is the effective dielectric constant from the effective medium approximation, and all ϵ_n (n=1,2,3,...) refer to the dielectric constant of individual components, V_n (n=1,2,3,...) are the volume fraction of the dielectric component and absorbing components.

The Maxwell-Garnett mixing rule assumes that a host material contains all other composite materials. The Maxwell-Garnett mixing rule is given by

$$\frac{\epsilon-\epsilon_1}{\epsilon+2\epsilon_1}=V_2\frac{\epsilon_2-\epsilon_1}{\epsilon_2+2\epsilon_1}+V_3\frac{\epsilon_3-\epsilon_1}{\epsilon_3+2\epsilon_1}+\ldots,\quad (V_1+V_2+V_3+\ldots=1), \tag{2}$$

where ϵ is the effective dielectric constant and ϵ_1 is the dielectric constant of the host material which contains all other composite materials.

The solution of the two-component Bruggeman mixing rule is

$$\epsilon=\frac{1}{4}\Big(\sqrt{\epsilon_1^2V_1(9V_1-6)+18\epsilon_1\epsilon_2V_1(1-V_1)+4\epsilon_1\epsilon_2+9\epsilon_1^2V_1^2-12\epsilon_2^2V_1^2+\epsilon_1^2+4\epsilon_2^2}+3\epsilon_1V_1-\epsilon_1-3\epsilon_2V_1+2\epsilon_2\Big). \tag{3}$$

The refractive index m can be obtained as $m=\sqrt{\epsilon}$.

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So far the Bruggeman mixing rule for two-component inclusions has been widely used [11–14]. In nature, multiple-component mixtures with more than two components are commonly existing. A typical example is the mixture of black carbon, organic carbon and sulfate aerosol [15–18]. In principle, Eq. (1) can be solved numerically for any number of inclusions through a reiteration. However, since the dielectric constant is a complex number, two loops of reiteration have to be applied to the real and imaginary parts of the dielectric constant separately, and this process is complicated and time-consuming. To our knowledge, the Bruggeman mixing rule has seldom been applied to the case of three components. Here we provide an analytical solution to Bruggeman mixing rule of three-component inclusions,

$$\epsilon = \frac{A_3}{6} - \frac{B}{12 \times 2^{1/3}} + \frac{D}{6 \times 2^{2/3} B}, \tag{4}$$

where $B = (A_1 + A_2 + A_4 + \sqrt{4D^3 + (A_1 + A_2 + A_4)^2})^{1/3}$,
$D = -4A_3^2 - 12A_5$;

$A_{1,2} = 72V_{1,2}(\epsilon_3^2(6\epsilon_3 V_{1,2}^2 - 12\epsilon_3 V_{1,2} + 8\epsilon_3 + 30\epsilon_1 V_{1,2} - 18\epsilon_1 V_{1,2}^2 - 3\epsilon_2 V_{1,2} - 10\epsilon_1 + 4\epsilon_2) + \epsilon_3(4\epsilon_1^2 - \epsilon_2^2) + \epsilon_1(2\epsilon_1\epsilon_2 - 2\epsilon_1^2 + \epsilon_2^2) + 6\epsilon_3\epsilon_1(3\epsilon_1 V_{1,2}^2 - 4\epsilon_1 V_{1,2} + \epsilon_2 V_{1,2} - \epsilon_2)) + 16\epsilon_1^2(1 - 27V_{1,2}^3) + 216\epsilon_1^2 V_{1,2}^2(2\epsilon_1 - \epsilon_2)$;

$A_3 = (3V_1 - 1)(\epsilon_1 - \epsilon_3) + (3V_2 - 1)(\epsilon_2 - \epsilon_3)$;

$A_4 = 216V_1V_2\epsilon_3(2\epsilon_3^2(3V_2 + 3V_1 - 4) - \epsilon_1^2 - \epsilon_2^2 - 10\epsilon_1\epsilon_2) + 216V_1V_2\epsilon_1\epsilon_2(\epsilon_1 + \epsilon_2 - 6\epsilon_1V_1 - 6\epsilon_2V_2) + 1296V_1V_2\epsilon_3((\epsilon_2^2 - \epsilon_1\epsilon_3 - 2\epsilon_2\epsilon_3 + 2\epsilon_1\epsilon_2)V_2 + (\epsilon_1^2 - \epsilon_2\epsilon_3 - 2\epsilon_3\epsilon_1 + 2\epsilon_1\epsilon_2)V_1) + 24(81V_1V_2\epsilon_3^2 - 4\epsilon_3^2 - \epsilon_1\epsilon_2)(\epsilon_1 + \epsilon_2) + 48\epsilon_3(\epsilon_1^2 + \epsilon_2^2) - 128\epsilon_3^3 - 192\epsilon_3\epsilon_1\epsilon_2$;

$A_5 = 3\epsilon_2V_1(\epsilon_1 - \epsilon_3) + 3\epsilon_1V_2(\epsilon_2 - \epsilon_3) + 2\epsilon_3(\epsilon_1 + \epsilon_2) - \epsilon_1\epsilon_2$.

For $V_1 = 0$ or $V_2 = 0$, the results of Eqs. (4) and (3) are identical.

The Maxwell-Garnett mixing rule is also widely used. For example, it is sometimes used for the calculation of optical properties of cloud droplets containing black carbon (BC) [19–23]. The solutions of the Maxwell-Garnett mixing rule are very simple,

$$\epsilon = \frac{(2a+1)\epsilon_1}{1-a} \tag{5}$$

where $a = V_2\frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + 2\epsilon_1}$ for a two-component mixture and $a = V_2\frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + 2\epsilon_1} + V_3\frac{\epsilon_3 - \epsilon_1}{\epsilon_3 + 2\epsilon_1}$ for a three-component mixture.

2. Model application

In the following, the Bruggeman mixing rule with three components is illustrated by applying to the atmospheric aerosols as sulfate aerosol (SO_4), BC and organic carbon (OC). These three aerosols are deemed important for climate change [24], and they are usually in internal mixing state [18,25–27]. A proper method to deal with the mixture of three aerosol is necessary.

For the mixture of SO_4, BC and OC, we denote the results of (4) as $(SO_4\text{+BC+OC})_B$ and (5) as $(SO_4\text{+BC+OC})_{MG}$. In $(SO_4\text{+BC+OC})_{MG}$, we take SO_4 as the host material. Also, the mixture can be calculated by the method of volume averages of the dielectric constants and volume averages of the refractive index, which are the mixing rules used occasionally in various applications. The effective dielectric constant by the volume averages of the dielectric constant is

$$\epsilon = V_1\epsilon_1 + V_2\epsilon_2 + (1 - V_1 - V_2)\epsilon_3, \tag{6}$$

and we denote this method as $(SO_4\text{+BC+OC})_\epsilon$. The effective refractive index by the volume averages of the refractive index is

$$m = V_1m_1 + V_2m_2 + (1 - V_1 - V_2)m_3, \tag{7}$$

and we denote this method as $(SO_4\text{+BC+OC})_m$. These results will be compared to the solutions of the Bruggeman and Maxwell-Garnett mixing rules.

For SO_4, we choose the refractive index of sulfate acid with 50% of volume water [28]. The refractive index of BC is from [29] and the refractive index of OC is from HITRAN 2012 database. The refractive index of sulfate acid, BC and OC are shown in Fig. 1.

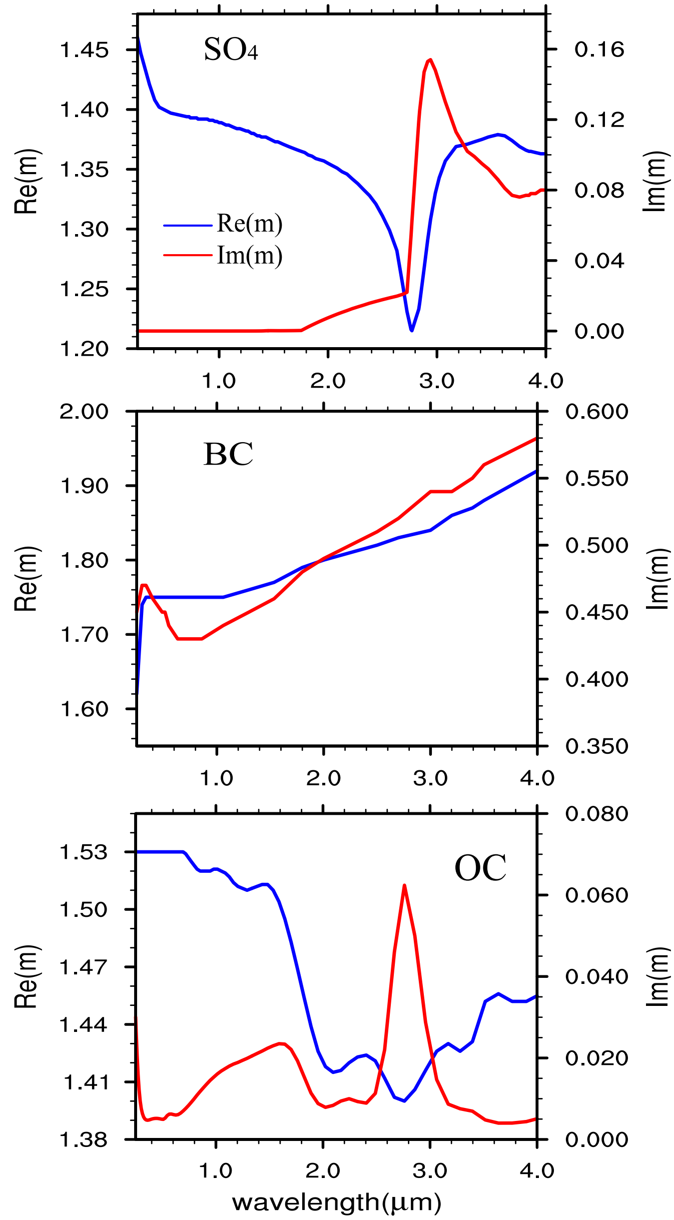

Fig. 1. The real and imaginary parts of the refractive index verse wavelength for SO_4, BC and OC. The OC refractive index is from ftp://cfa-ftp.harvard.edu/pub/HITRAN2012/Aerosols-2016/ascii/single_files.

The results of the effective refractive index by various methods are shown in Fig. 2. The volume fractions of OC (V_{OC}) are set to 0.2, the volume fractions of SO_4 (V_{SO_4}) are set to 0.3, 0.5 and 0.7, and the volume fraction of BC (V_{BC}) is $1 - V_S - V_{OC}$. We choose the volume fractions of SO_4 changing from small to large, as the chance increases for the host material containing all other composite materials.

The top panels of Fig. 2 show that the real part of the refractive index of $(SO_4\text{+BC+OC})_B$ is generally larger than those of $(SO_4\text{+BC+OC})_\epsilon$ and $(SO_4\text{+BC+OC})_m$ but becomes smaller in the range of 2.8–4.0 µm. The Bruggeman mixing rule handles the real and imaginary parts of refractive index together, which is very different from the method of volume average schemes, which treat the two parts separately. The values of $(SO_4\text{+BC+OC})_{MG}$ are obviously larger than those of $(SO_4\text{+BC+OC})_B$ when the volume frac-