



Investigations of Radiative Properties Estimated from Rayleigh and Mie Scattering Theories

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Abstract

Radiative properties are very important parameters for the numerical simulation of thermal radiation transfer through porous medium. To estimate the radiative properties of the porous medium, Mie and Rayleigh scattering theories are usually preferred to compute the radiative properties of a single sphere, and applied for estimating the radiative properties of a porous media. But, there are some limitations. Therefore, in this work we have investigated the differences of radiative properties computed by these two scattering theories. The results shown that, for a very small sphere, there are no significant differences in radiative properties computed from Rayleigh and Mie scattering theories. But, for a particle size larger than 1/10 of the radiation wavelength, Mie scattering is preferred. The spectral transmittances of porous mediums made from different materials that the radiative properties were estimated from Rayleigh and Mie scattering theories have also been simulated and reported.

Keywords: Mie scattering / Rayleigh scattering / Radiative properties / Porous medium.

1. Introduction

In the thermal radiative transfer problems at nano-scale, it is frequently solved by numerical methods. One of the most effective methods is the Monte Carlo method which can be applied for complicated boundary conditions that are difficult to analyze using radiative transport equation [1]. The Monte Carlo simulation of light propagation through porous medium or tissues was modeled [2], the radiative properties of the medium or tissue can be estimated using the theory of light scattering by small particles [3, 4], by this way, the

radiative properties of a single particle can be determined. For the medium, especially the porous medium, the radiative properties namely absorption and scattering coefficients (K_{abs} and K_{sca}) usually can be computed using independent scattering approximation, and applies the radiative properties of a single particle to determine the radiative properties of a participating media. In order to compute the absorption and scattering coefficients of a single particle, Mie and Rayleigh scattering theories are usually selected. The Rayleigh scattering is originally formulated, applicable to small,



dielectric (non-absorbing), spherical particle. For the Mie scattering, it is generally applicable for spherical scattering as well as Rayleigh scattering. However, Rayleigh scattering theory is generally preferred if applicable, due to the complexity of the Mie scattering formulation. But, there are some advantages and disadvantages for Rayleigh and Mie scattering Theories. Therefore, this study presents the radiative properties of particles and mediums that were estimated from Mie and Rayleigh scattering theories, comparisons, and the advantage and disadvantage of these two scattering theories.

2. Theory

2.1 Rayleigh scattering theory

Rayleigh scattering theory is expressed the scattering of light by particles that much smaller than the wavelength of light (λ). It occurs when light travels in transparent solids, liquids and gases [5]. The two parameters that absolutely important in determination of the radiative properties of the medium are the scattering and extinction efficiencies (Q_{sca} and Q_{ext}). The calculation using Rayleigh scattering theory can be done from

$$Q_{sca} = \frac{3}{8} \left| \frac{m^2 - 1}{m^2 + 2} \right|^2 x^4 \quad (1)$$

$$Q_{ext} = -4 \operatorname{Im} \left\{ \frac{m^2 - 1}{m^2 + 2} \right\} x \quad (2)$$

when m is the complex index of refraction ($m = n - ik$), and x is the size parameter which can be calculated from $x = 2\pi a/\lambda$, a is a radius of particle.

2.2 Mie scattering theory

Mie's scattering occurs when the particles are the same size or slightly larger than the wavelength of radiation in contact with them.

Gustave Mie first obtained a solution for the scattering of plane waves from a sphere when the spheres diameter is slightly larger than the wavelength of light. The scattering and extinction efficiencies (Q_{sca} and Q_{ext}) can be calculated using [5]

$$Q_{sca} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) (|a_n|^2 + |b_n|^2) \quad (3)$$

$$Q_{ext} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}\{a_n + b_n\} \quad (4)$$

where a_n and b_n are referred to the Mie scattering coefficients, can be calculated from

$$a_n = \frac{\psi'_n(y)\psi_n(x) - m\psi_n(y)\psi'_n(x)}{\psi'_n(y)\zeta_n(x) - m\psi_n(y)\zeta'_n(x)} \quad (5)$$

$$b_n = \frac{m\psi'_n(y)\psi_n(x) - \psi_n(y)\psi'_n(x)}{m\psi'_n(y)\zeta_n(x) - \psi_n(y)\zeta'_n(x)} \quad (6)$$

where $y = mx$, and the functions ψ_n and ζ_n are known as Reccati – Bessel functions, and are defined in terms of half-integer-order Bessel function of the first kind ($J_{n+1/2}(z)$), where

$$\psi_n(z) = \left(\frac{\pi z}{2} \right)^{1/2} J_{n+1/2}(z) \quad (7)$$

$$\zeta_n(z) = \left(\frac{\pi z}{2} \right)^{1/2} H_{n+1/2}(z) \quad (8)$$

where $H_{n+1/2}(z)$ is the half-integer-order Henkel function of the second kind.

2.3 Absorption and scattering cross-sections

The amount of absorption and scattering by a particle is usually expressed in terms of the absorption cross-section, C_{abs} , and scattering cross-section, C_{sca} , that are related to the total amount of absorption and scattering [6], or extinction cross-section as,

$$C_{ext} = C_{abs} + C_{sca} \quad (9)$$

From the absorption and scattering efficiency factors of a particle that can be calculated by Rayleigh and Mie theories, and its



projected area of the sphere, the absorption and scattering cross-sections can be calculated from

$$C_{abs} = Q_{abs} \cdot \pi a^2 \quad (10)$$

$$C_{sca} = Q_{sca} \cdot \pi a^2 \quad (11)$$

where the absorption efficiency, can be calculated from relationship,

$$Q_{ext} = Q_{abs} + Q_{sca} \quad (12)$$

2.4 Absorption and scattering coefficients

If the absorbing particles are suspended in an absorbing continuous medium, or composed to be a porous medium, then the absorption and scattering coefficients can be calculated from [6]

$$K_{abs} = C_{abs} \cdot N_0 \quad (13)$$

$$K_{sca} = C_{sca} \cdot N_0 \quad (14)$$

where N_0 is the number of density that related to the particle volume fraction, f_v , and the particle diameter, d . The number of density is calculated from

$$N_0 = \frac{f_v}{\frac{\pi}{6} d^3} \quad (15)$$

From the absorption cross-section and scattering cross-section that can be calculated according the projected area of particle, πa^2 , which is equal to $\pi d^2/4$. Therefore, the absorption and scattering coefficients can be reduced to

$$K_{abs} = C_{abs} \cdot N_0 = \frac{1.5Q_{abs} \cdot f_v}{d} \quad (16)$$

$$K_{sca} = C_{sca} \cdot N_0 = \frac{1.5Q_{sca} \cdot f_v}{d} \quad (17)$$

2.5 Scattering phase function

When light strikes a particle with an index of refraction different from its environment, the light is refracted. The angle at which the light is bent is a function of the size and shape of the particle as well as the wavelength of the incident light and the incidence angle of the light. In

general, each particle will have a different scattering profile. This scattering profile is called the phase function. Henyey and Greenstein [7] introduced a function that just varies one parameter in the range of $-1 \leq g \leq 1$, in which ranges from backscattering through isotropic scattering to forward scattering. The function is

$$P_{HG}(\theta) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - 2g \cos(\theta))^{3/2}} \quad (18)$$

where $P_{HG}(\theta)$ is a probability density function, θ is the angle existing between the direction of the photon before a scattering event and the direction after the scattering event. The parameter g is defined as

$$g = \cos(\theta) = \int_0^\pi \cos(\theta) P_{HG}(\theta) 2\pi \sin(\theta) d\theta \quad (19)$$

The value of $g = 1$ means the photon carries on in the same direction as before the collision. If the value of $g = 0$ means the photon has the same probability of going in any direction. From the originally proposed by Witt [8], the Eq. (18) is slightly modified as

$$P_{HG}(\cos(\theta)) = \frac{1}{2} \frac{1 - g^2}{(1 + g^2 - 2g \cos(\theta))^{3/2}} \quad (20)$$

And the distribution of $P_{HG}(\theta)$ can be generated from

$$\int_{-1}^{\cos(\theta)} P_{HG}(\cos(\theta')) d(\cos(\theta')) = \xi \quad (21)$$

And the exact analytical solution for of Eq. (21) can be expressed as

$$\cos(\theta) = \begin{cases} \frac{1}{2g} \left[1 + g^2 - \left(\frac{1 - g^2}{1 - g + 2g\xi} \right)^2 \right], & \text{if } g \neq 0 \\ 2\xi - 1, & \text{if } g = 0 \end{cases} \quad (22)$$

where ξ is the uniformly distributed random number.

3. Modeling and Simulation

3.1 Modeling of the porous mediums

In this study, the nano-size spherical shape materials namely; titanium dioxide (TiO_2), silicon dioxide (SiO_2), and yttrium oxide (Y_2O_3) were chosen for modeling and used in simulations. It was assumed that the shapes of these materials are perfectly spherical and uniform size. The radiative properties of these three types of materials were calculated based on Rayleigh and Mie scattering theories that have been expressed previously for their differences investigation. The details of the single spherical particles are shown in Table. 1.

Based on these three types of materials, three types of porous mediums were modeled. In these models, the porous mediums were ideally assumed that their porous structures can be formed by compose many nano-size single spherical materials to be a thin film with nano-porous structure as shown in Fig. 1. The details of porous mediums were also shown in Table. 2.

Table. 1 Details of the single spherical particles and their refractive indices at the wavelength of 1000 nm

Materials	Particle size, nm	Refractive index, n
TiO_2	Vary from 1 to 1000	2.4856 (High n)
Y_2O_3	Vary from 1 to 1000	1.9029 (Medium n)
SiO_2	Vary from 1 to 1000	1.5351 (Low n)

Table. 2 Details of the three porous mediums

Materials	Particle size, nm	f_v	Thickness, μm
TiO_2	10, 100, 200	0.3	10
SiO_2	10, 100, 200	0.3	10
Y_2O_3	10, 100, 200	0.3	10

Table. 3 Refractive indices of materials [9,10]

Wavelength, nm	TiO_2	SiO_2	Y_2O_3
400	2.5304	1.5577	1.9822
500	2.5045	1.5488	1.9471
600	2.4954	1.5438	1.9289
700	2.4910	1.5407	1.9182
800	2.4884	1.5384	1.9113
900	2.4867	1.5366	1.9065
1000	2.4856	1.5351	1.9029

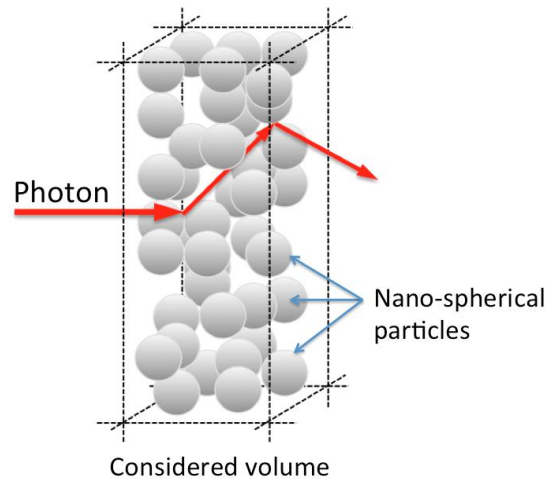


Fig. 1 Model of a nano-porous medium

3.2 Numerical simulation of radiative transfer

To solve the radiative transfer problems, there are many means of approximating radiative transfer; Monte Carlo method is one of the most popular methods for Radiative Transfer simulations. In this study, the radiative properties calculated from the previous expression were used to estimate the radiative properties of the three types of mediums as have been mentioned in 3.1. After that, simulations of the photons transport through these three types of the mediums were performed based on the Monte

Carlo method [11]. The schematic of the photons transport through the medium was also shown in Fig 2.

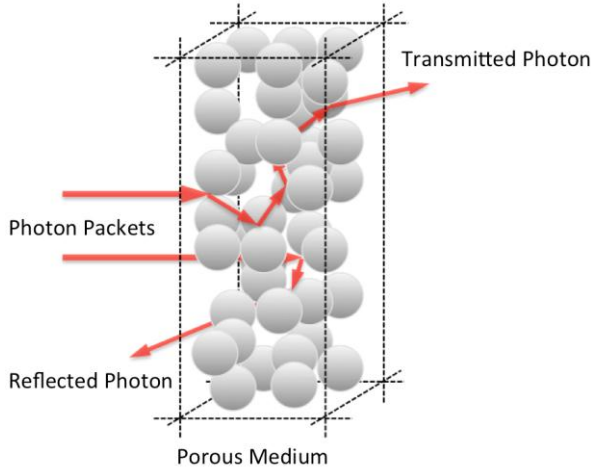


Fig. 2 Schematic of the photons transport through the porous medium

4. Results

In this work, we have compared the radiative properties of various sizes of single spherical particles that were computed from Rayleigh and Mie scattering theories. The simulated spectral transmittance of the modeled porous mediums were also shown as followings,

4.1 Single spherical particles

For the radiative properties of the single spherical particles, in this work we focused on the differences of scattering efficiencies of various sized single spherical particles that were computed from Rayleigh and Mie scattering theories.

From the scattering efficiencies of the three different materials shown in Fig. 3, the computation parameters were used in the simulation are shown in Table. 1. The results reveal that, at small particle sizes, especially for smaller than 300 nm, the scattering efficiencies calculated from Rayleigh and Mie theories were

not obviously different between them. But, for large particle sizes, especially for larger than 300 nm, the scattering efficiencies in which calculated from Rayleigh were increased as much as increasing of the particle sizes. And the differences between them were increasing rapidly especially for scattering efficiencies which calculated from Rayleigh theory. Also the different of scattering efficiency was caused by the different of refractive index.

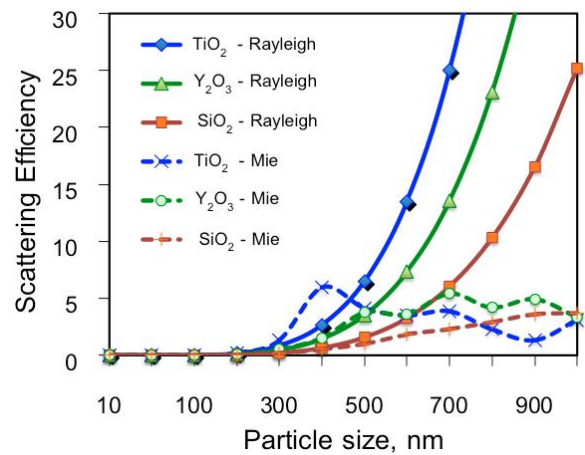


Fig. 3 Scattering efficiencies of various sizes of single spherical TiO₂ particles computed from Rayleigh and Mie scattering theories.

Table. 3 Percentage of different in scattering efficiencies computed from Rayleigh and Mie scattering theories at constant wavelength 1 μm

Size parameter, x	Particle size, nm	Percentage of Difference, %		
		High n (TiO ₂)	Medium n (Y ₂ O ₃)	Low n (SiO ₂)
0.0031	1	0.0006	0.0003	0.0001
0.0157	5	0.015	0.009	0.002
0.0314	10	0.061	0.034	0.010
0.1571	50	1.522	0.851	0.236
0.3142	100	6.193	3.355	0.862
1.5708	500	36.472	6.207	36.195
3.1416	1000	97.006	94.095	85.315

To compare the differences of scattering efficiencies calculated from Rayleigh and Mie theories in term of size parameter, x , Table. 3 is shown that, for small x , percentage of the difference was very small, but, for large x (x around 1 and higher), percentage of the difference was rapidly increased. From Table. 3, it can be concluded that the differences of radiative properties computed from Rayleigh and Mie scattering theories were dominantly affected by the size of particles with the wavelength of radiation. Also depending on the refractive index of materials, lower refractive index at the same size parameter gave lower percentage of difference.

4.2 Porous mediums

In this section, the porous mediums that have been expressed in section 3.2 were considered. The mediums were investigated by simulating the photons transport through their porous structures. Each medium was ideally made from each material; there were 3 sizes of particles, namely 10 nm, 100 nm, and 200 nm in diameter, with constant thickness of 10 μm . However, in this simulation, we could not perform the simulation for the medium in which made from the particle size larger than 200 nm. Because the radiative properties of the medium computed from Rayleigh scattering theory were very large values and caused the simulator to run infinite loop.

In order to estimate the radiative properties of each medium, the radiative properties of single particles which calculated from Rayleigh and Mie scattering theories were applied for participating media as have been expressed in section 2.4. In this study, we

focused on the spectral transmittances that were simulated for each medium, and compare to each other in which having the same material, but different particle sizes and different scattering theories of radiative property calculation.

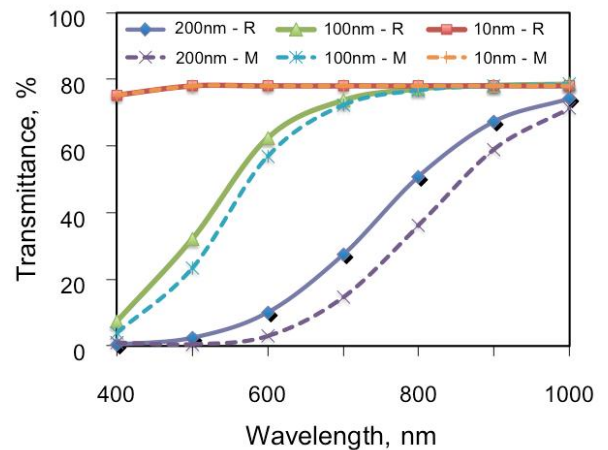


Fig. 4 Spectral transmittances of porous mediums made from various sizes of TiO_2 particles, their radiative properties were computed from Rayleigh (R) and Mie (M) scattering theories.

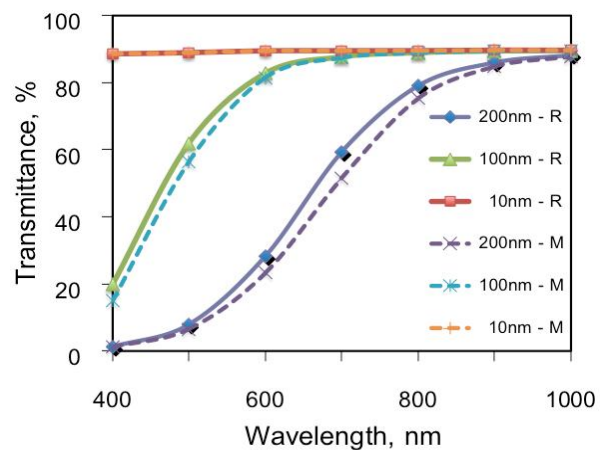


Fig. 5 Spectral transmittances of porous mediums made from various sizes of Y_2O_2 particles, their radiative properties were computed from Rayleigh (R) and Mie (M) scattering theories.

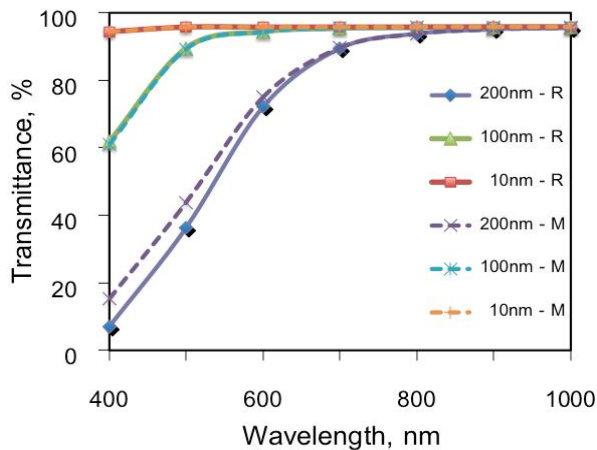


Fig. 6 Spectral transmittances of porous mediums made from various sizes of SiO_2 particles, their radiative properties were computed from Rayleigh (R) and Mie (M) scattering theories.

As the results of simulated spectral transmittances were shown in Figs. 4, 5, 6, we can see that for the shorter radiation wavelength and larger particle size, the transmittance will be low. In the other hand, for longer radiation wavelength with smaller particle size, the transmittance will be high. These were agreed with the other measurement data that generally can be seen in material handbooks [12].

In order we consider the results of spectral transmittance based on particle sizes, it was clearly that for small particle size (10 nm, red and dotted orange lines) the spectral transmittance curves that were simulated based on Rayleigh and Mie scattering theories look no difference between them, and gave the same results for all three medium types. In this case of smallest particle size, the mediums were highest transmittance if compare to the other particle sizes. Otherwise, the medium which made from SiO_2 material was highest transmittance when compared to the other materials.

For medium particle size (100 nm, green and dotted green lines), the spectral transmittance curves that were simulated based on Rayleigh and Mie scattering theories look similar tendency between them for each medium. But, if consider based on their different refractive index, the medium which made from low refractive index material (SiO_2), their spectral transmittances were not different between them. Otherwise, with the same consideration, the medium which made from higher refractive index materials (TiO_2 and Y_2O_3), the spectral transmittance curves were slightly different between them.

For large particle size (200 nm, purple and dotted purple lines), the spectral transmittance curves based on Rayleigh and Mie scattering theories were highest different between them, especially for higher refractive index material (TiO_2), the spectral transmittance curves show obviously different between them.

In order we consider the difference of spectral transmittance between scattering theories, because Rayleigh and Mie scattering theories gave different radiative properties of a single particle. Therefore, the radiative properties of the medium that estimated from these different radiative properties will also be different. But, large or small difference will be upon the particle sizes.

5. Conclusions

In this work, we have showed the differences of radiative properties of single particles that were computed from Rayleigh and Mie scattering theories. We found that, for small particle or small size parameter (x), their results were obviously not different. But, for large



particle or large size parameter, their results were obviously different associated with the increasing of particle size.

For the porous mediums, their radiative properties were estimated from Rayleigh and Mie scattering theories the results were shown that for small particles of porous structure, the spectral transmittances were similarly. But, for large particles of porous structure, the spectral transmittances became obviously different. These were because the Rayleigh can give accurate radiative properties just for very small particles. Anyway, because Rayleigh scattering formulation is very short and simple, this is the advantage point of using the Rayleigh scattering theory to estimate the radiative properties of particles.

The advantage of Mie scattering theory is that the radiative properties of any particle size can be determined. Otherwise, the disadvantage of Mie scattering theory is that the complexity of its formulation. In order to determine the radiative properties of particles or mediums by Rayleigh or Mie theories, it is very important to check for the suitable size parameter. From our investigations, it is suggested that Rayleigh scattering could be applied for radiative property determination if the particle size is not exceed than 1/10 of the radiation wavelength.

7. References

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