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REPRESENTATIONS OF TRANSITION MATRIX COEFFICIENTS FOR THE GENERALIZED LORENTZ MIE SCATTERING CALCULATIONS

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ABSTRACT

With uncertainty in changing global and regional climate variations, it has become important to obtain accurate quantitative computation on particle's radiative properties. Transition matrix method (T- Matrix) is one of the powerful tool for the Mie computations for light scattering and absorptions coefficients by isotropic particles is presented. The internal $\vec{E}^{(inc)}(r)$ and scattered $\vec{E}^{(sca)}(r)$ fields are approximated by the vector spherical wave functions $M_{mn}(kr)$ and $N_{mn}(kr)$. Considering the linearization of the Maxwell equations and the constitutive relations, the $\vec{E}^{(sca)}(r)$, $\vec{E}^{(inc)}(r)$ and the scattering characteristics were computed. When the particle is spherical and in nonmagnetic media, all the non-zero T-matrix elements are diagonal, such that $(Q^{pq})^{12}_{mn,m_1n_1} = (Q^{pq})^{21}_{mn,m_1n_1} = 0$. Hence, all the Lorentz Mie scattering coefficients are derived and computed for some various particle parameters. It was found that, the T- matrix technique is applicable to a wide range of particle's scattering parameters.

Key words: Maxwell equations, Transition matrix, Mie theory, scattering coefficients,

INTRODUCTION

The theories and numerical computations of light scattering by particles (spherical and inhomogeneous) have found many applications in atmospheric sciences, astronomy, engineering, chemistry and biophysics. However, the uncertainties in light scattering characteristics upon interaction with particles attract the attentions of many researchers, since it was first conceived by P.C. Waterman. (Waterman 1965) and recently developed over last three decades (Barber and Hill 1990), (Borghese *et al.*, 2003), Chew (1994), Doicu *et al.*, 2000, 2006), Mishchenko *et al.*, (2000). With current challenges in changing climate modelling, it is important to obtain reliable and accurate quantitative information on particles parameters such as atmospheric aerosol optical properties on a global scale. This paper aimed for the alternative derivation of Mie scattering coefficients by spherical particles using the T- matrix technique. This technique can be applied to any symmetric or asymmetric particles. The unique feature of the T-matrix depends on the geometrical and physical characteristics of the particle and is independent on the propagation direction and polarization states of the incident and scattered field.

THEORETICAL FORMULATION

The general behavior of the macroscopic field in any given media is described by Maxwell's equations in differential forms; (Doicu *et al.*, 2006).

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (1)$$

$$\nabla \times \vec{H} = J + \frac{\partial \vec{D}}{\partial t} \quad (2)$$

$\nabla \cdot \vec{D} = \rho$ (3)

$\nabla \cdot \vec{B} = 0$ (4)

Where $\vec{B}$ is the magnetic induction, $\vec{E}$ and $\vec{H}$ are the electric and magnetic fields, $\vec{D}$ is the electric displacement and ρ and $\vec{J}$ the electric charge density and current density respectively.
The T- matrix relates the expansion coefficients of the incident and scattered fields due to series expansions of the incident and scattered fields. The scattered and incident fields in terms of radiating vector spherical wave functions are given to be (Doicu *et al.*, 2006);

$$\mathbf{E}^{(sca)}(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} f_{mn} M^{3}_{mn}(k_s\mathbf{r}) + g_{mn}\mathbf{N}^{3}_{mn}(k_s\mathbf{r}) \quad (5)$$

$$\mathbf{E}^{(inc)}(\mathbf{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{mn} M^{1}_{mn}(k_s\mathbf{r}) + b_{mn}\mathbf{N}^{1}_{mn}(k_s\mathbf{r}) \quad (6)$$

From equations (5) and (6) the functions f_{mn} *and* g_{mn} and a_{mn} *and* b_{mn} are related in matrix form, known as transition matrix (**T** - matrix) as;

$$\begin{bmatrix} f_{mn} \\ g_{mn} \end{bmatrix} = \mathbf{T}\begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} = \begin{bmatrix} \mathbf{T}^{(11)} & \mathbf{T}^{(12)} \\ \mathbf{T}^{(21)} & \mathbf{T}^{(22)} \end{bmatrix}\begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} \quad (7)$$

The leading diagonal components, $\mathbf{T}^{(11)}$ and $\mathbf{T}^{(22)}$,describe the transformation with the same parity (electric to electric and magnetic to magnetic), while the off diagonal components, $\mathbf{T}^{(12)}$ and $\mathbf{T}^{(21)}$ describe the coupling between different parity (electric to magnetic and magnetic to electric).

If the T- matrix is known, all the scattering characteristics such as *extinction, scattering and absorption cross section* can be readily computed.

In terms of the expansion coefficients $a_{mn}, b_{mn} f_{mn}$ *and* g_{mn}. The extinction and scattering cross section can be expressed as (Bingqiang *et al.*, 2020; Doicu *et al.*, 2006)

$$C^{(ext)} = -\mathrm{Re}\left\{\frac{j\pi R}{k_s}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}(f_{mn}a^{*}_{mn} + g_{mn}b^{*}_{mn}\right\}\times \left\{\begin{matrix} h^{(1)}_{n}(k_sR)\left[k_s j_n R(k_sR)\right]' - \\ j_n(k_sR)\left[k_sRh^{(1)}_{n}(k_sR)\right]')\end{matrix}\right\} \quad (8a)$$

Using the Wroskian relation (Doicu *et al.*, 2006),

$$h^{(1)}_{n}(k_sR)_n\left[k_sRj(k_sR)\right]' - j_n(k_sR)\left[k_sRh^{(1)}_{n}(k_sR)\right]' = -\frac{j}{k_sR} \quad (8b)$$

then

$$C^{(ext)} = -\frac{\pi}{k_s^2}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\mathrm{Re}(f_{mn}a^{*}_{mn} + g_{mn}b^{*}_{mn}) \quad (9)$$

LORENTZ MIE THEORY

For isotropic particle, the T-matrix relating the expansion coefficients of the scattered and incident fields is given by the Q^{pq} matrices $(p = \theta, \phi)$ for the e_r- dependency and $(q = \beta, \alpha)$ are for the e_k- dependency. On relating the particle's coordinate system, the expressions for the incident and scattered fields are

$$E^{(inc)}\left(r,\theta,\varphi\right)=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}a_{mn}M_{mn}^{1}\left(k_s,r,\theta,\varphi\right)+b_{mn}N_{mn}^{1}\left(k_s,r,\theta,\varphi\right) \qquad (10)$$

$$E^{(sca)}\left(r,\theta,\varphi\right)=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}f_{mn}M_{mn}^{3}\left(k_s,r,\theta,\varphi\right)+g_{mn}N_{mn}^{3}\left(k_s,r,\theta,\varphi\right) \qquad (11)$$

While in the global coordinate system, these expansions take the form

$$E^{(inc)}\left(r,\Phi,\Psi\right)=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\tilde{a}_{mn}M_{mn}^{1}\left(k_s,r,\Phi,\Psi\right)+\tilde{b}_{mn}N_{mn}^{1}\left(k_s,r,\Phi,\Psi\right) \qquad (12)$$

$$E^{(sca)}\left(r,\Phi,\Psi\right)=\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\tilde{f}_{mn}M_{mn}^{3}\left(k_s,r,\Phi,\Psi\right)+\tilde{g}_{mn}N_{mn}^{3}\left(k_s,r,\Phi,\Psi\right) \qquad (13)$$

When the media is nonmagnetic, then;

$k_1=k_0\sqrt{\varepsilon_1}$, $k_2=k_0\sqrt{\varepsilon_2}$ and the matrix $Q^{pq}(k_1,k_2)$ takes the form (Doicu *et al.*, 2006),

$$Q^{pq}(k_1,k_2)=\begin{bmatrix}\left(Q^{pq}\right)^{11} & \left(Q^{pq}\right)^{12}\\ \left(Q^{pq}\right)^{21} & \left(Q^{pq}\right)^{22}\end{bmatrix} \qquad (14)$$

Such that.

$$\left(Q^{pq}\right)^{11}=\frac{jk_1^2}{\pi}\int_S\left\{\left[n(r')\times M^q(k_2r')\right]\cdot N^p(k_1r')+\sqrt{\frac{\varepsilon_2}{\varepsilon_1}}\left[n(r')\times N^q(k_2r')\right]\cdot M^p(k_1r')\right\}dS(r') \qquad (15)$$

$$\left(Q^{pq}\right)^{12}=\frac{jk_1^2}{\pi}\int_S\left\{\left[n(r')\times N^q(k_2r')\right]\cdot N^p(k_1r')+\sqrt{\frac{\varepsilon_2}{\varepsilon_1}}\left[n(r')\times M^q(k_2r')\right]\cdot M^p(k_1r')\right\}dS(r') \qquad (16)$$

$$\left(Q^{pq}\right)^{21}=\frac{jk_1^2}{\pi}\int_S\left\{\left[n(r')\times M^q(k_2r')\right]\cdot M^p(k_1r')+\sqrt{\frac{\varepsilon_2}{\varepsilon_1}}\left[n(r')\times N^q(k_2r')\right]\cdot N^p(k_1r')\right\}dS(r') \qquad (17)$$

$$\left(Q^{pq}\right)^{22}=\frac{jk_1^2}{\pi}\int_S\left\{\left[n(r')\times N^q(k_2r')\right]\cdot M^p(k_1r')+\sqrt{\frac{\varepsilon_2}{\varepsilon_1}}\left[n(r')\times M^q(k_2r')\right]\cdot N^p(k_1r')\right\}dS(r') \qquad (18)$$

The Lorenz–Mie theory shows that, the Q^{pq} matrices equation (14) are diagonal such that:

$$(Q^{pq})_{mn,m_1n_1}^{12}=(Q^{pq})_{mn,m_1n_1}^{21}=0 \qquad (19)$$

For all such values of m,n,m_1 *and* n_1. Therefore,

$$(Q^{31})_{mn,m_1n_1}^{11}=jx\left\{j_n(m_rx)[xh_n^{(1)}(x)]'-h_n^{(1)}(x)m_rxj_n(m_rx)]'\right\}\delta_{mm_1}\delta_{nn_1} \qquad (20)$$

$$(Q^{33})^{11}_{mn,m_1n_1} = jx\left\{h_n^{(1)}(m_rx)[xh_n^{(1)}(x)]' - h_n^{(1)}(x)[m_rxh_n^{(1)}(m_rx)]'\right\}\delta_{mm_1}\delta_{nn_1} \quad (21)$$

$$(Q^{11})^{11}_{mn,m_1n_1} = jx\left\{j_n(m_rx)[xj_n(x)]' - j_n(x)[m_rxj_n(m_rx)]'\right\}\delta_{mm_1}\delta_{nn_1} \quad (22)$$

$$(Q^{13})^{11}_{mn,m_1n_1} = jx\left\{h_n^{(1)}(m_rx)[xj_n(x)]' - j_n(x)[m_rxh_n^{(1)}(m_rx)]'\right\}\delta_{mm_1}\delta_{nn_1} \quad (23)$$

$$(Q^{31})^{22}_{mn,m_1n_1} = \frac{jx}{m_r}\left\{-h_n^{(1)}(x)[m_rxj_n(m_rx)]' + m_r^2 j_n(m_rx)[xh_n^{(1)}(x)]'\right\}\delta_{mm_1}\delta_{nn_1} \quad (24)$$

$$(Q^{11})^{22}_{mn,m_1n_1} = \frac{jx}{m_r}\left\{-j_n(x)[m_rxj_n(m_rx)[xj_n(x)]' + m_r^2 j_n(m_rx)[xj_n(x)]'\right\}\delta_{mm_1}\delta_{nn_1} \quad (25)$$

$$(Q^{13})^{22}_{mn,m_1n_1} = \frac{jx}{m_r}\left\{-j_n(x)[m_rxh_n^{(1)}(m_rx)[xj_n(x)]' + m_r^2 h_n^{(1)}(m_rx)[xj_n(x)]'\right\}\delta_{mm_1}\delta_{nn_1} \quad (26)$$

$$(Q^{33})^{22}_{mn,m_1n_1} = \frac{jx}{m_r}\left\{-h_n^{(1)}(x)[m_rxh_n^{(1)}(m_rx)]' + m_r^2 h_n^{(1)}(m_rx)[xh_n^{(1)}(x)]'\right\}\delta_{mm_1}\delta_{nn_1} \quad (27)$$

Where $x = k_sR$ is the size parameter and $m_r = \sqrt{n_i / n_s}$ is the relative refractive index of the particle with respect to the ambient medium. For suitable computing the Q^{pq} matrices take the logarithmic derivatives of A_n *and* B_n by;

$$A_n(x) = \frac{d}{dx}\left\{\ln[xj_n(x)]\right\} = \frac{[xj_n(x)]'}{xj_n(x)} \quad (28)$$

And

$$B_n(x) = \frac{d}{dx}\left\{\ln[xh_n^{(1)}(x)]\right\} = \frac{[xh_n^{(1)}(x)]'}{xh_n^{(1)}(x)} \quad (29)$$

Using the recurrence relation

$$[xz_n(x)]' = xz_{n-1}(x) - nz_n(x) \quad (30)$$

Where z_n stands for j_n *or* $h_n^{(1)}$ then, equations (21) – (28) can be written as

$$(Q^{31})^{11}_{mn,m_1n_1} = -jx^2(m_rx)\left\{[m_rA_n(m_rx) + \frac{n}{x}]h_n^{(1)}(x) - h_{n-1}^{(1)}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (31)$$

$$(Q^{31})^{22}_{mn,m_1n_1} = -jm_rx^2 j_n(m_rx)\left\{[\frac{A_n(m_rx)}{m_r} + \frac{n}{x}]h_n^{(1)}(x) - h_{n-1}^{(1)}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (32)$$

$$(Q^{33})^{11}_{mn,m_1n_1} = -jx^2h_n^{(1)}(m_rx)\left\{[m_rB_n(m_rx) + \frac{n}{x}]h_n^{(1)}(x) - h_{n-1}^{(1)}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (33)$$

$$(Q^{33})^{22}_{mn,m_1n_1} = -jm_r x^2 h_n^{(1)}(m_r x)\left\{[\frac{B_n(m_r x)}{m_r} + \frac{n}{x}]h_n^{(1)}(x) - h_{n-1}^{(1)}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (34)$$

$$(Q^{11})^{11}_{mn,m_1n_1} = -jx^2 j_n(m_r x)\left\{[m_r A_n(m_r x) + \frac{n}{x}]j_n(x) - j_{n-1}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (35)$$

$$(Q^{11})^{22}_{mn,m_1n_1} = -jx^2 h_n^{(1)} j_n(m_r x)\left\{[\frac{A_n(m_r x)}{m_r} + \frac{n}{x}]j_n(x) - h_{n-1}^{(1)}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (36)$$

$$(Q^{13})^{11}_{mn,m_1n_1} = -jx^2 h_n^{(1)}(m_r x)\left\{[m_r B_n(m_r x) + \frac{n}{x}]j_n(x) - j_{n-1}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (37)$$

$$(Q^{13})^{22}_{mn,m_1n_1} = -jm_r x^2 h_n^{(1)}(m_r x)\left\{[\frac{B_n(m_r x)}{m_r} + \frac{n}{x}]j_n(x) - j_{n-1}(x)\right\}\delta_{mm_1}\delta_{nn_1}, \quad (38)$$

COMPUTATIONAL TECHNIQUE

The functions $\Psi_n(x) = \frac{n+1}{x} - \frac{1}{\Psi_{n+1}(x) + \frac{n+1}{x}}$ (39) Where Ψ_n stands for A_n *and* B_n such that stable scheme for computing Ψ_n relies on the estimate of Ψ_n, where n is larger than the number of terms required for convergence.

The T matrix for spherical particle is diagonal with entries

$$T^{11}_{mn,m_1n_1} = T_n^1 \delta_{mm_1,nn_1} \quad (40)$$

and

$$T^{22}_{mn,m_1n_1} = T_n^2 \delta_{mm_1,nn_1} \quad (41)$$

Where

$$T_n^1 = -\frac{[m_r A_n(m_r x) + \frac{n}{x}]j_n(x) - j_{n-1}(x)}{[m_r A_n(m_r x) + \frac{n}{x}]h_n^{(1)}(x) - h_{n-1}^{(1)}(x)} \quad (42)$$

$$T_n^2 = -\frac{[\frac{A_n(m_r x)}{m_r} + \frac{n}{x}]j_n(x) - j_{n-1}(x)}{[\frac{A_n(m_r x)}{m_r} + \frac{n}{x}]h_n^{(1)}(x) - h_{n-1}^{(1)}(x)} \quad (43)$$

Equations (43) and (44) relate the T- matrix to the size parameter x and relative refractive index m_r .

The data extracted using the software package TMATRIX FORTRAN program to compute the scattering and absorption of electromagnetic waves by particles with arbitrary geometries using the T- matrix method developed by Doicu for various particle's parameters (Doicu *et al.*, 2006);

RESULT AND DISCUSSION

The results were computed using continental polluted aerosols as particles under considerations.

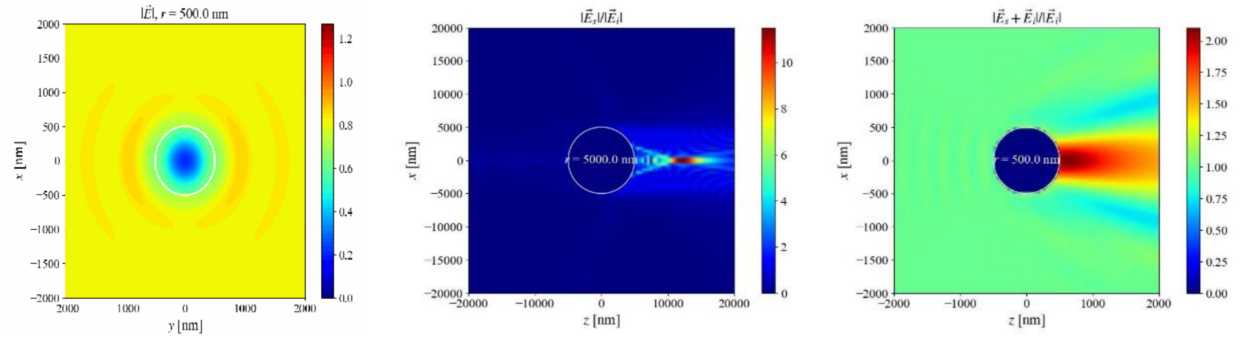
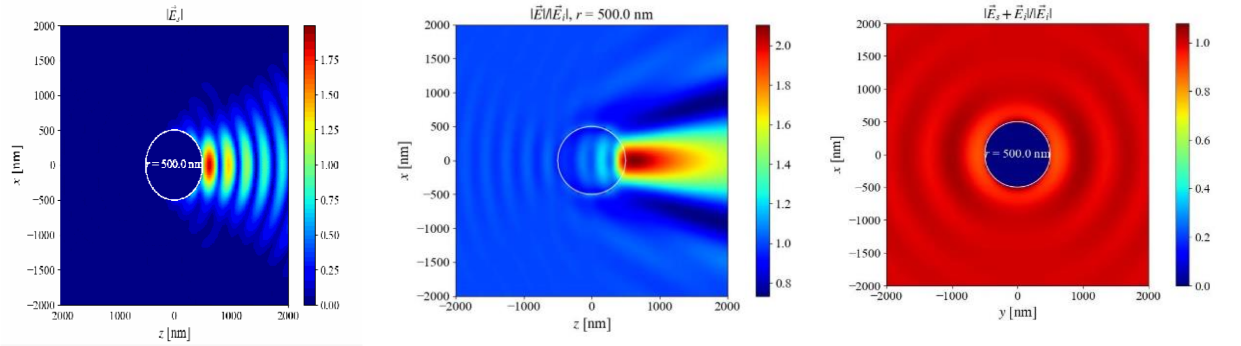


Figure 4.1(a) (b) (c)



(d) (e) (f)

Figure 4.1(a) – (f) shows the near field amplitudes of scattered electric field intensity at the wavelength of 323 nm inside a continental polluted aerosols of radius 5000 nm, n = 1.64 + 0.0i .

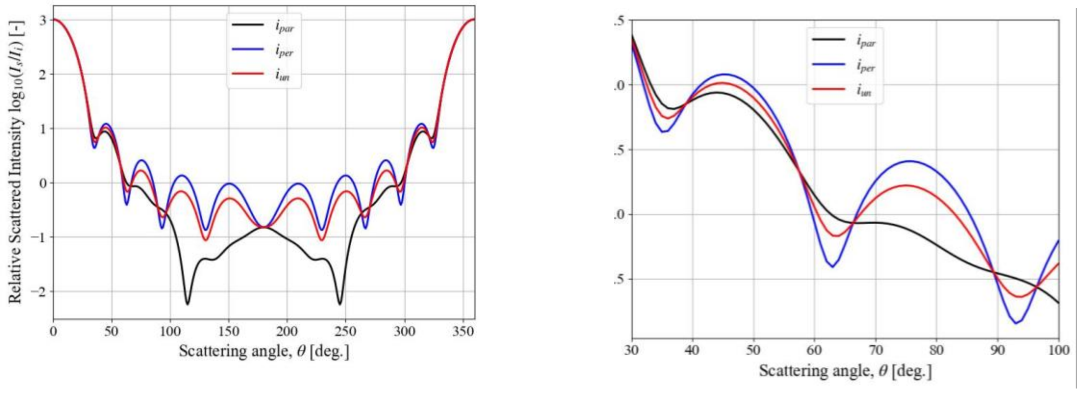
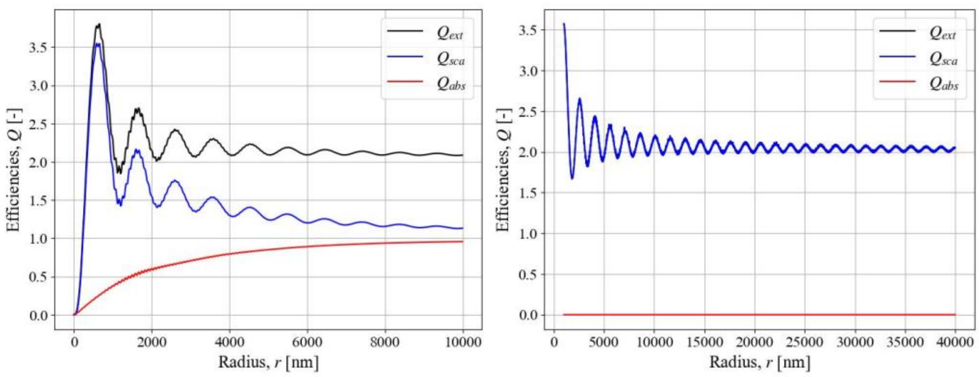
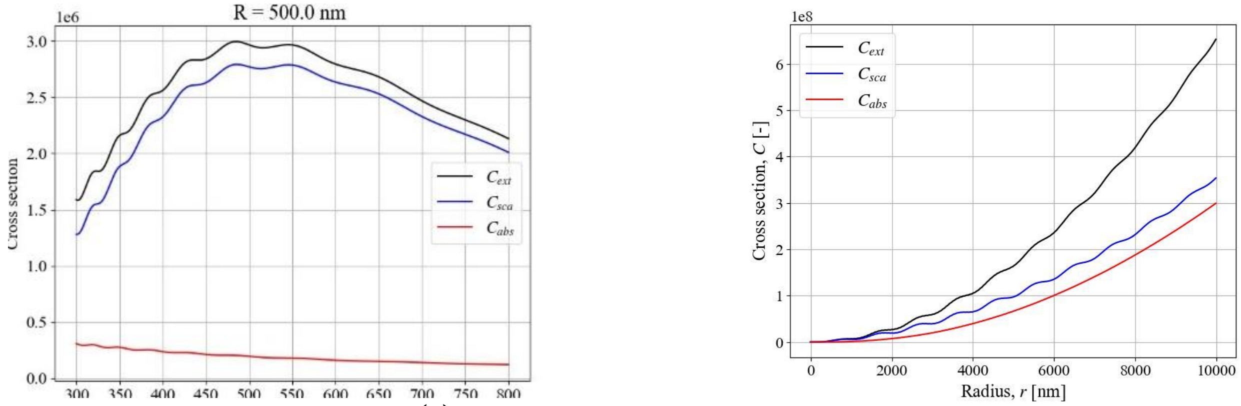


Figure 4.2 (a) and (b), presents the variations relative scattering intensity with scatting angles wavelength of 323 nm inside a continental polluted aerosols of radius 5000 nm, n = 1.64 + 0.0i.



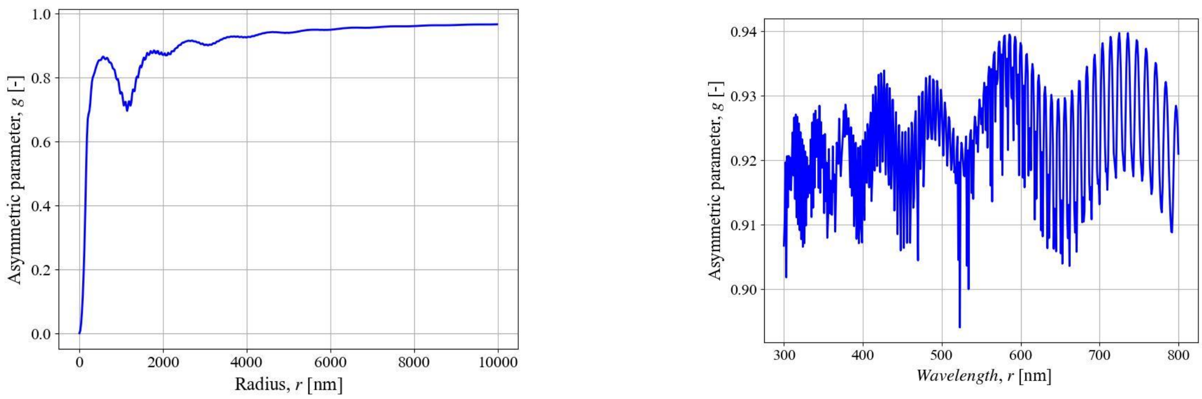
(a) (b)

Figure 4.3 (a) and (b), presents the variations efficiency factor with particles' radius at wavelength of 323 nm inside a continental polluted aerosols of radius 5000 nm, n = 1.64 + 0.0i.



(a) (b)

Figure 4.4 (a) and (b),show the variations in scattering cross section with particles' radius at wavelength of 323 nm inside a continental polluted aerosols of radius 5000 nm, n = 1.64 + 0.0i.



(a) (b)

Figure 4.5 and show the variations in asymmetry factors with particles'(a) radius at (b) wavelength inside a continental polluted aerosols of radius 5000 nm, n = 1.64 + 0.0i.

CONCLUSION

The Lorenz Mie theory of interaction between electromagnetic radiations and a spherically homogeneous particle has been studied within the framework of T-matrix formalism. The Lorentz Mei scattering coefficients are readily derived in terms of T-matrix. The derivation provides an opportunity to investigate the applicability of Lorentz Mie coefficients and to make recommendations for future research. It has been found that, the T- matrix method is applicable to a wide range of particle's scattering parameters such as wide range particle's radius, wavelengths and refractive indices.

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