Extended geometrical optics approximation and Monte Carlo ray tracing for light scattering by an irregular object

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Abstract
The extended geometrical optics approximation (EGOA) and the Monte Carlo ray tracing (MCRT) have been improved to include more scattering effects and used to explore the light scattering by a spheroidal droplet and bubble. The EGOA method takes into account not only deviation of each light ray and the divergence/convergence of ray bundle, but also the interferences between rays, the diffraction, the absorption and the incident beam profile. It has been extended to the oblique incidence case and used to study the light scattering of a plane wave by a spheroidal droplet or bubble of arbitrary ellipticity. The MCRT method can treat scattering by objects of any shape in 3D. The existed model has been improved by taking into account the interferences, absorption, polarization of the incident wave and its beam shape. The comparison of the two methods has been made for each aforementioned effect and the agreement is found always very good. It is also shown that the scattering patterns of a spheroidal bubble are quite different from those of a spheroidal droplet. High dependence of ellipticity on the scattering intensity is found for a spheroidal droplet.

1. Introduction

In order to increase energy efficiency and reduce pollutant emissions, it is essential to study the combustion processes in automobile, aircraft or other industrial engines. The optical metrology techniques are widely used to investigate and control these processes because of its non-intrusive nature, fast (or real-time) response, robust sensitivity and versatility. To invent new measurement techniques and improve existed techniques for flow characterization, rigorous theories and approximate methods describing the interaction of light with particles have been developed. The Lorenz-Mie theory (LMT) (Bohren and Huffman 1983) and the generalized Lorenz-Mie theory (GLMT) (Gouesbet and Grehan 2000) provide rigorous solutions to the problem of light scattering by a particle of simple shape (sphere, cylinder…) illuminated by a laser beam. They are widely applied to improve optical measurement techniques: phase Doppler anemometry, rainbow refractometry, digital holography, etc. However the particles encountered in two-phase flows are not always of simple shape. For example, the atomization process does not give instantaneously spherical droplets, but large non-spherical droplets: liquid ligaments and filaments which are intermediate states. The rigorous theories are no longer valid since they are limited to particles of regular form.

To resolve this problem, several approximate theories have been established to treat light scattering by irregular objects. For example, the T-matrix has been developed by Mishchenko et al. (1997) for scattering of nonspherical particles. Nousiainen and Muinonen (2007) have explored the surface-roughness effects on single-scattering properties of wavelength-scale particles with the discrete-dipole approximation (DDA) and the finite-difference time domain method (FDTD) was employed by Yang and Liou (1996) for light scattering by small ice crystals in three-dimensional space …

We are interested in two other methods: the extended geometrical optics approximation (EGOA) and the Monte Carlo ray tracing (MCRT). The former method is extended on the base of geometrical optics theory which is widely used for analysis and calculations of optical problems.
due to its calculation efficiency and clear interpretation of scattering mechanism. The on-axis Gaussian beam scattering by a spherical particle and by a spheroidal particle with end-on incidence have been studied by Xu et al. (2006, 2006). The MCRT method is a flexible and powerful tool taking into account complex configurations for simulation of single and multiple scattering by large non-spherical particles (Mikrenska and Koulev 2009).

The aims of present work have been 1). to extend the EGOA method to non-axis-symmetric illumination case: the particle is illuminated by an inclined wave and 2). to include in the MCRT model different effects in the interaction between the photons and the particle. Furthermore, when we treat the scattering of particles of relatively complex shape (a spheroid here), no rigorous theory is available to compare. The two models we use permit to validate each other.

This paper is organized as follows: in section 2 we describe briefly the two methods and the extension we have done. The comparisons of the numerical results predicted by these two methods are then presented in section 3 and finally, conclusions are given in Section 4.

2. Description of the two methods

We describe in this section the two models (EGOA and MCRT) and the improvements we have done for the simulation of the interaction of light with complex shape particles.

The geometrical optics approximation (GOA) is on the basis of van de Hulst’s (1957) discussions. From the point view of GOA, the incident beam is composed of many individual light rays. The amplitude and the phase of each ray of different order can be calculated numerically in versus of scattering angles when a ray suffers external reflection, refraction and several times of internal reflections. The times of experienced internal reflection are used to distinguish ray order. Then the total scattering field can be obtained by a superposition of the complex amplitude of the different order rays and the diffracted field (Xu et al. 2006, 2006). This improved model takes into account not only deviation of each light ray and the divergence/convergence of the ray bundle, but also the interferences between different modes in considering of all the phase shifts (due to ray path and focal lines), the effects of diffraction, absorption and the incident beam profile. Considering all these effects, it has been proved that the EGOA can correctly predict the scattering patterns of simple cases explored by the rigorous theories. However, the first version of EGOA is limited to the 2D axis-symmetric case where the scattering pattern is symmetric between 0 and ±180°. In order to extend the EGOA to oblique incident case, we have taken into account the incident angle in the ray tracing and the phase difference due to the oblique incidence. The scattering pattern is calculated from 0° to 360°.

The MCRT model, on the other hand, can treat the scattering by an object of arbitrary shape in 3D illumined by a wave. It allows defining a very general shape of the particle: a 3D function $f(\vec{x}), \vec{x} \in R^3$ is created representing the distance of any point $\vec{x}$ in the space to the surface of the particle. In other terms, the particle surface is the level set of function $f$ corresponding to zero. The function $f$ is given on each point of mesh, similarly to the result of some fluid mechanics computations (Tanguy et al. 2007). The MCRT consists in sending photons from a side of the mesh, and to compute their intersections with the particle surface. In order to obtain the accurate position of the intersection between a given photon and the particle surface, a 3D interpolation of $f$ is computed inside each cell (Lekien and J. Marsden 2005). As is known, the interaction of a photon with a facet of the particle surface may result in new photon: refracted photon or reflected photon. Therefore, each time when a photon encounters the particle surface, refraction or reflection will be determined by the comparison of a uniformly distributed random number from 0 to 1 with the Fresnel coefficient. This numerical approach is flexible and it has great capabilities to simulate multiple scattering in optically dense random media (Xu 2004; Calba et al. 2006; Rozé et al. 2008). But the effects of polarization, diffraction, absorption and interferences as well as the incident beam
shape have not been taken into account in the original version. Usually, the absorption was accounted for by means of stochastic procedures (Takano and Liou 1995; Kirk 1992): the transmission associated with an actual path length will be compared with a random number and the absorption or the transmission of a photon will be determined. Here, we just multiple the transmission which denotes the portion of transmitted energy with the weight of a photon to take into consideration the absorption. Similarly, the two polarization components and their corresponding phases (Serikov and Kawamoto 2001) will be carried by photons in our MCRT model. So that each simulated photon will be traced with a complex amplitude which serves to study the polarization and the interference between photons. For the incident beam shape, the Gaussian beam has been introduced as the way of Xu et al. (2006, 2006): the amplitude and the phase which describe the incident Gaussian beam will be given to each photon whereas it hits the particle surface for the first time. The amplitude is given directly by the electric field expression of the Gaussian beam and the incident direction is determined according to the normal of the wave front. Moreover, the diffraction effect will be taken into account by the Heisenberg uncertainty ray bending model (Serikov and Kawamoto 2001) which can count the diffraction of each photon for various shapes of apertures/particles (Heinisch and Chou 1971).

3. Numerical results

On the basis of the methods described in the above section, codes are realised in FORTRAN language to simulate the scattering diagrams of a spheroidal droplet and bubble illuminated by a plane wave or a Gaussian beam. Fig. 1 and 2 show the scattering patterns calculated by the EGOA respectively for a spheroidal droplet and bubble of different ellipticities illuminated by a plane wave. We can find that the scattering diagrams of the spheroidal droplets are very sensible to the ellipticity, but not for spheroidal bubbles. Precisely, the position of rainbow angle varies with the ellipticity. By comparing these two figures, an obvious difference of scattering patterns between spheroidal droplets and spheroidal bubbles is observed.

![Fig. 1 Scattering intensities calculated by EGOA for a spheroidal droplet of transversal radius b = 100µm, symmetric axis a = 200µm, 110µm, 95µm, 50µm and of relative refractive index m = 1.33 illuminated by a non-polarized plane wave of wavelength λ = 0.6328µm. The curves of a = 110µm, 95µm, 50µm have been offset relatively by the factors of 10³, 10⁶ and 10⁹ for clarity](image_url)
The EGOA has also been extended to non-axis-symmetric incident beam case. Fig. 3 and 4 show the scattering diagrams of a spheroid illuminated by a plane wave with different incident angles. The scattering patterns vary with the incident angle. With an increase of incident angle, we can find that there is a remarkable backward movement of the primary rainbow position for a spheroidal droplet.

On the other hand, the MCRT model has been extended by adding the effects of absorption, polarization, incident beam shape and interferences. To validate the model, the basic scattering case of a sphere illuminated by a plane wave has been studied for each added effect by comparison with EOGA.

First of all, to study the absorption effect, we consider an unpolarized plane wave illuminating a particle and we do not take into account the interference between different rays. Fig. 5 shows the normalized intensity distributions simulated by the two models for an absorbing sphere with different imaginary parts of the refractive index. We find that the agreement between the two methods is very good. The little difference is due to the limited of photon number in MCRT ($10^9$ photons for the curves in Figs. 5 and 6).
Fig. 4 Same parameters as Fig. 3, but for a spheroidal bubble of relative refractive index $m = 0.75$.

Fig. 5 Comparisons of the scattering intensities calculated by EGOA and by MCRT for absorbing sphere of radius $a = 50\mu m$ and refractive index $m = (1.33, 0.001)$ and $m = (1.33, 0.0005)$ illuminated by a non-polarized plane wave of wavelength $\lambda = 0.6328 \mu m$. The interferences and the diffraction are not taken into account.

Then in Fig. 6 we show the scattering intensities of a sphere illuminated by a polarized plane wave and we find again the agreement between the two models is very good except near $0^\circ$ and $180^\circ$ where there is a singularity in MCRT. If the above mentioned effects are counted in the simulation, both the EGOA and the MCRT agree well with the Mie theory (Fig. 7). The agreement of the results predicted by the two models and by Mie theory is found very good in general. Nevertheless, a remarkable discrepancy is discerned near $0^\circ$ since the diffraction has not been taken into account.

Fig. 6 Comparisons of the scattering intensities calculated by EGOA and by MCRT for a sphere of radius $a = 50\mu m$ and of refractive index $m = 1.33$ illuminated by a polarized plane wave of wavelength $\lambda = 0.6328 \mu m$.
Since our perspective is to predict the scattering of an arbitrary shaped beam by an irregular object, we should study the scattering of a non-plane wave. The Gaussian beam is the simplest non-plane wave which permits to introduce the incident beam profile in our models. The intensity distributions of each ray order calculated by EGOA and by MCRT for a sphere illuminated by a Gaussian beam are shown in Fig. 8. It is clearly seen that the contributions of each mode are very different when the particle is illuminated by a Gaussian beam of radius less than that of the sphere. For example, the contributions of the reflection to the small angle and the rainbow picks are no longer visible since the incident Gaussian beam is centered on the axis of the particle and the intensity near the border is very weak. For the case shown in Fig 8.b, the amplitude of electric field is less than $10^{-2}$ at the position of rays which contribute to the first order of rainbow.

As mentioned before, there is no rigorous theory available for the scattering of for a large spheroid. The EGOA and the MCRT we developed permit to verified the numerical results each other. We show in the following the scattering diagrams simulated by the two models for a spheroidal droplet and a spheroidal bubble.

The scattering diagrams of a spheroidal droplet of transversal radius $b = 25\mu m$, symmetric radius $a = 50\mu m$ and a spheroidal bubble of the same parameters are shown in Fig. 9 and 10. The incident polarized plane wave is along the symmetric axis of the spheroid. We find that the results of the EGOA correspond well to those of the MCRT accept in the zone between 50° and 70°. Further investigation is to be done to reveal the reason. It should be pointed out that the diffraction effect has not been counted in this simulation.
Fig. 9 Comparisons of the scattering intensities of a spheroidal droplet of transversal radius \( b = 25\,\mu m \), symmetric radius \( a = 50\,\mu m \) and of refractive index \( m = 1.33 \) illuminated by a polarized plane wave of wavelength \( \lambda = 0.6328\mu m \) calculated by EGOA and by MCRT.

Fig. 10 Same parameters as Fig. 9, but for a spheroidal bubble of relative refractive index \( m = 0.75 \)

For taking into consideration the diffraction effect, we intend to employ the Heisenberg uncertainty ray bending model (Serikov et al 2001) in our MCRT model. We simulated the diffraction of a slit by this method and we find a good agreement between simulated diffracted field and the results calculated by the analytical expression (Fig. 11). It is believed that this flexible model is suitable to study the diffraction for object of any shape. The diffraction effect for a spheroid in non-axis-symmetric illumination case is still under study.

Fig. 11 Comparisons of the scattering intensities for diffraction field calculated by analytical diffraction expressions and by MCRT for a slit of width \( a = 10\,\lambda \) illuminated by a plane wave of wavelength \( \lambda = 0.6328\mu m \)
4. Conclusion

In this paper, two models of scattering by an irregular object have been improved and used for light scattering by a spheroid: the extended geometrical optics approximation and the Monte Carlo ray tracing. The EGOA has been extended to a spheroidal particle (droplet and bubble) of any ellipticity for non axisymmetric case. The interferences, absorption, polarization and the incident beam shape have taken into account in the MCRT model. All the effects have been validated by comparisons with the EGOA results for a sphere. It is shown that the two models can predict well the scattering diagram in all direction from 0 to 360° and the results of the two models agree well when the same effects are taken into account.

It is shown that the scattering patterns of a spheroidal bubble are very different from that of a spheroidal droplet because of different scattering mechanisms. An evident dependence of ellipticity on the scattering diagram is found for a spheroidal droplet but not for a spheroidal bubble. For the oblique illumination case, the scattering patterns of a spheroid are sensible to the incident angle.

As near perspectives, the improvement of these two models will allow us to predict accurately the light scattering by an irregular object in 3D which will be very useful for spray imaging and other optical metrology techniques. It will lead to a better understanding of present optical diagnosis and innovation in spray metrology.

References

Bohren CF, Huffman DR (1983) Absorption and Scattering of Light by Small Particles.


Van de Hulst HC (1957) Light Scattering by Small Particle. Wiley Edt


