Introducing phase tracing into a computational method which combines ray-tracing with diffraction on facets

Evelyn Hesse¹, Zbigniew Ulanowski¹, Adrian J.M. Clarke¹, Stephan Havemann², and Paul H.Kaye¹

¹ Science and Technology Research Center, University of Hertfordshire, Hatfield, AL10 9AB, UK ² Met Office, Cordouan2, C2-5, Fitzroy Road, Exeter, EX1 3PB, UK tel: +44-1707-28-5251, fax: +44-1707-28-4185, e-mail: E.Hesse@herts.ac.uk

Abstract

The viability of introducing phase tracing into our ray tracing with diffraction on facets model is investigated. In order to prove the method, Monte Carlo ray-tracing results for a slit, based on our diffraction formula and including phase, are compared with the Fraunhofer diffraction formula. In a next step, light scattering results obtained with this method for a long conducting column and a long dielectric column with square cross section are compared with SVM.

1. Introduction

The importance of ice and mixed-phase clouds to the earth-atmosphere radiation balance and climate is well established. Yet, present understanding of cirrus with regard to scattering properties of ice crystals is weak, which is partly due to inadequate theoretical models. For realistic crystal shapes and sizes accurate models either do not exist, have not yet been adequately verified or are computationally very demanding, especially for larger size parameters. A modified Kirchhoff approximation (MKA) method has been introduced [1] to calculate far fields from classical geometric optics (GO) results, which encouraged the development of the improved GO model [2]. The latter is however computationally expensive. For moderate values of the size parameter the finite difference time domain (FDTD) method can be used [3] but it puts even more severe demands on computational resources. Thus, despite its limitations, geometric optics (GO) combined with projected-area diffraction [4] is still the most widely used model for moderate to large size parameters. Therefore, substantial improvement in the theory of scattering on ice crystals is important if phenomena such as radiative forcing by cirrus are to be understood and the sign and magnitude of cirrus cloud-climate feedback established. Recently, diffraction on facet has been introduced into a ray tracing model [5], [6], and a 3D-version will be presented at this conference [7]. Phase function and other elements of the scattering matrix are significantly improved. In the work shown here, the viability of introducing phase tracing into the geometric optics code combined with diffraction on facets is tested.

2. Computational method 2.1. General considerations

Based on the concept of energy flow lines, in the ray-tracing combined with diffraction on facets code [5-7] each ray reflected or refracted at a crystal facet is deflected towards the nearest edge according to

$$\varphi = \arctan\left(\frac{\lambda}{4\pi^2} \left(\frac{1}{x} - \frac{1}{2a - x}\right)\right) \tag{1}$$

where φ is the deflection angle, λ the wavelength, *x* the distance from the nearest edge, and 2*a* the projection of the facet width into the plane perpendicular to the ray. In this paper, we modify the above assumption in such a way, that two reflected and refracted rays are created at each point where a ray hits the crystal surface (except for total internal reflection). With respect to classical ray-tracing, one of the rays is deflected towards the nearest edge according to eq. (1), and the other one is deflected towards the far edge by the same amount. The concept of beam-splitting is based on the necessity to conserve momentum. For a black half plane it can be shown that there is a phase shift of π between

rays refracted at angles $\pm \varphi$ with respect to the direction of the incident beam after subtracting the incident field [8]. Following this result we assume that the two refracted beams have a phase shift of π with respect to each other and a phase shift of $\pm \pi/2$ with respect to the original beam. Considering that for the black half plane the above consideration is also true for scattering angles larger than 90° (measured from the forward direction), we apply the same phase relations to the two reflected rays. In order to limit the number of rays which have to be traced, randomly one of the two beams is chosen for ray tracing, and the other one disregarded. We first test this concept for diffraction on a slit.

2.2. Diffraction on a slit

Fig. 1 shows the intensity distribution for diffraction on a 10 μ m slit, λ =514.5nm, calculated using ray-tracing combined with diffraction according to eq.(1) with and without phase-tracing, and the Fraunhofer diffraction formula. We use cylinder coordinates, and all results are normalized according to

$$\frac{1}{\pi} \int_{-\pi/2}^{\pi/2} d\theta p_{11cyl}(\theta) = 1$$
 (2)

where θ is the angle with the incident direction in the equatorial plane, and p_{11cyl} is the corresponding phase function. The bin size is 0.1°. The interference pattern created by Monte Carlo ray-tracing including phase agrees well with the Fraunhofer diffraction pattern. Only very close to the direct forward scattering direction, i.e.



Fig.1: Diffraction on a 10 μ m slit: Fraunhofer diffraction and Monte Carlo ray tracing according to eq.(1).

between 0 and 0.2° , the Monte Carlo results deviate from the Fraunhofer pattern, as is to be expected from the introduced phase shift of π between the two diffracted rays into which each incoming ray is split. However, this deviation is very small, as can also be seen from the good agreement of the intensities at the maxima after normalization. The improvement with respect to Monte Carlo raytracing without phase tracing is significant. Therefore, the introduction of phase tracing into the raytracing combined with diffraction on facets program is expected to be a major improvement.

2.3. Diffraction on long column with square cross section

The crystal geometry which is most similar to a slit, and which is therefore considered most suitable to test the model is a long column with square cross section and perpendicular incident of the light rays onto one of its long facets. In order to simplify the scattering problem by eliminating any refraction, at first a conducting column is considered. In the following, our phase tracing model is tested against the Separation of Variables Method (SVM) [9,10].

2.3.1. Conducting column

Fig. 2 shows the scattering pattern calculated by SVM for perpendicular incidence onto a rectangular facet of a conducting square column (edge length $l = 20\lambda/\pi$), and the Fraunhofer diffraction pattern for a slit of width $20\lambda/\pi$. The Fraunhofer diffraction pattern is mirrored at $\theta = 90^{\circ}$, so that the backscattering $(180\pm90)^{\circ}$ is identical to the forward scattering $(0\pm90)^{\circ}$. We find a very good agreement between the SVM-result and the Fraunhofer pattern in the backscattering half-circle, particularly in the region $(180\pm60)^{\circ}$. This confirms that reflection can be modelled by using the same beam splitting

procedure as described in section 2.2. for diffraction on a slit. The oscillations near 90°, which continue towards smaller scattering angles, are most likely due to scattering from the facets parallel to the incident rays. There is good agreement for the central diffraction peak around the forward direction $(0\pm7)^{\circ}$. We find that better agreement for the first minimum and the second maximum from the forward direction can be obtained by including externally diffracted rays into the Monte Carlo calculation. For this purpose, the width of the acceptance area for incident rays is extended from the width *l* of the square cross section towards 21. This is a rough approximation based on extinction cross section of two. an External rays are deflected towards and away from the nearest edge in the same way as for a half plane:

$$\varphi = \pm \arctan\left(\frac{\lambda}{4\pi^2 x}\right) \tag{3}$$



Fig.2: SVM-result for perpendicular incidence on a conducting long square cylinder of edge length 40, $\lambda = 2 \pi$ and Fraunhofer diffraction pattern for a slit of width 40, and Monte Carlo ray tracing with phase at an obstacle of

where x is the distance from the nearest edge. Due to the fast decay of deflection angle with increasing distance from the column, the central maximum is too high. These are contemporary results. First tests showed, that it is feasible to correct the amplitude of the central maximum by introducing correction terms, which come into effect for large distances x. On the other hand, phase tracing without including external rays improves the general shape of the phase function, and it improves backscattering significantly. Therefore, it is potentially useful for applications like the interpretation of lidar data.

2.3.2. Dielectric column

Fig. 3 shows the scattering pattern for a dielectric column with refractive index 1.31 calculated by SVM and ray-tracing with and without phase. Here, ray-tracing does not include external rays. Only for external reflection or outward refraction a phase shift of π between the two beams was introduced. As for the conducting column, phase tracing improves in the backscattering (180±50)°. Scattering in this region is mainly due to one external reflection, and therefore most straight forward for modelling. These are temporary results, and further investigations for multiple ray - crystal surface interactions are under way. In this respect, it would be useful to have the opportunity to test the model against proved results for larger size parameters.



Fig.3: SVM and ray-tracing with diffraction on facets results with and without phase tracing for perpendicular incidence on a long square cylinder of edge length 40, n=1.31, $\lambda = 2\pi$.

3. Conclusions

For a slit, we have compared Monte Carlo ray-inclusive phase-tracing results based on our diffraction formula with Fraunhofer diffraction and found good agreement. The improvement compared to the same ray-tracing method, but without phase-tracing, is significant. In a next step, light scattering results obtained with this method for a long conducting column and a long dielectric column with square cross section ($l = 20\lambda/\pi$) and perpendicular incidence onto one rectangular facet were compared with SVM. For the conducting column we found very good agreement in the backscattering half circle and for the central diffraction peak around the forward direction (0 ± 7)°. An improvement of the position of the first diffraction minimum and second maximum could be obtained by including externally diffracted rays. However, the treatment of external rays for larger distances from the particle, and the size of the projected area around the particle to be covered by ray-tracing need further investigation, since the calculated forward scattering peak is too high. For the dielectric column we find good agreement for backscattering. These are temporary results, and further investigations for multiple ray - crystal surface interactions are under way. In this respect, it would be useful if the model could be tested against proved results for larger size parameters, than are currently available from SVM.

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