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RADIATIVE PROPERTIES OF VISIBLE AND SUBVISIBLE CIRRUS: SCATTERING ON HEXAGONAL ICE CRYSTALS

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1. Introduction

One of the main objectives of the First International Satellite Cloud Climatology Project (ISCCP) Regional Experiment (FIRE) is to provide a better understanding of the physics of upper level clouds. There are a number of factors that have complicated the study of these clouds leaving our present understanding of upper level clouds in a less than satisfactory state. One factor is simply the distance of the clouds from the surface. It is easier to study a low-level cloud system because of their proximity to the ground. Added to this observational problem is the fact that clouds in the upper troposphere seem to be governed by an intricate balance of not so well understood phenomena. Among the factors that have added to the complexity of the problem is the fact that particles are no longer spherical and both the solid and liquid water phases may coexist. Turbulence develops in the stable layer environment with its fine scales of vertical motion. Horizontal eddies (two dimensional turbulence) may be important for cloud morphology, and a host of interactions between gravity waves, turbulence, radiation, and microphysics all seem possible.

This paper concentrates on just one specific aspect of cirrus physics, namely on characterizing the radiative properties of single, nonspherical ice particles. While focused in this way, this study provides the basis for further more extensive studies of the radiative transfer through upper level clouds. Radiation provides a potential mechanism for strong feedback between the divergence of in-cloud radiative flux and the cloud microphysics and ultimately on the dynamics of the cloud.

We will firstly describe some aspects of ice cloud microphysics that are relevant to the radiation calculations. Next, the Discrete Dipole Approximation (DDA) is introduced and some new results of scattering by irregular crystals are presented. We also adopt the Anomalous Diffraction Theory (ADT) to investigate the scattering properties of even larger crystals. In this way we are able to determine the scattering properties of non spherical particles over a range of particle sizes. The study reported here is still preliminary and at the time of writing this abstract, the results are incomplete. We aim to incorporate the microphysics data collected during FIRE into these calculations and in a companion study plan to use these scattering properties to determine cloud radiative heating rates.

2. Cloud microphysics

Characterizing the shape and size of ice crystals in terms of their environment continues to be a subject of extensive research. For environments typical of cirrus clouds and for even the colder environments of polar stratospheric clouds (PSC's), ice exists in single- and polycrystalline forms. The more commonly perceived large composite crystals, of the order of $500\mu m$, are actually observed more readily at lower temperatures. Crystal sizes of the order of $10\mu m$ and $1\mu m$ are, respectively, more representative of high cirrus in the tropics (Heymsfield, 1986) and PSC's (Rosen *et al.*, 1988). To emphasize this point we present the variation of crystal shape drawn in proportion to their size in Fig. 1 over the temperature range -20^oC to -90^oC. The crystals at cirrus temperatures, say -40^oC, are hexagonal columns although variations of this type of crystal exist in the form of hexagonal bullets and hollow columns. In this study we will focus only on single solid hexagonal crystals although the foundation to study crystals of more complex shape has been developed.

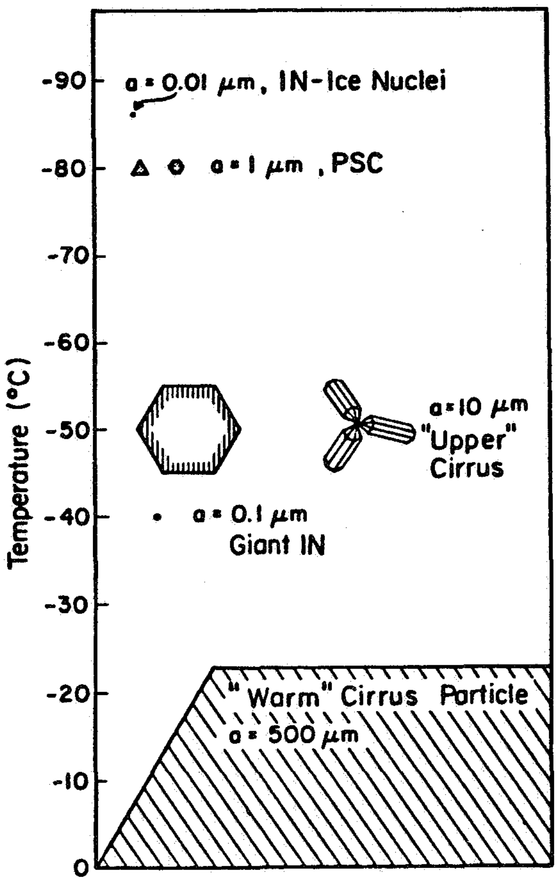

Fig. 1 *Typical sizes of ice crystals encountered in the temperature range* $(-20,-90)\,°C$. *The crystal sizes are approximately drawn to scale. Notice that the warm cirrus particle (all hatched in the low part of the diagram) is so large that only part is presented.*

3. Integral formulation of Maxwell equations and its approximation

Only a very brief outline of the scattering methods are described here. We begin with Maxwell equations written in the integral form (Saxon, 1955)

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}_0(\mathbf{x}) + 4\pi k^2 \times \int \mathbf{G}(\mathbf{x},\mathbf{x}') \cdot \frac{\epsilon(\mathbf{x}') - \mathbf{1}}{4\pi} \cdot \mathbf{E}(\mathbf{x}')\, d^3\mathbf{x}' \tag{1}$$

where $\mathbf{E}_0(\mathbf{x})$ is the incident electric field, $\epsilon(\mathbf{x})$ is a dielectric tensor, and Green's function is defined as

$$\mathbf{G}(\mathbf{x},\mathbf{x}') = (\mathbf{1} - \hat{\mathbf{r}}\hat{\mathbf{r}})\frac{e^{ikr}}{4\pi r} + (3\hat{\mathbf{r}}\hat{\mathbf{r}} - \mathbf{1})\left(\frac{1}{k^2r^2} - \frac{i}{kr}\right)\frac{e^{ikr}}{4\pi r} \tag{2}$$

where $\mathbf{r} = \mathbf{x} - \mathbf{x}'$, $r = |\mathbf{x} - \mathbf{x}'|$, and $\hat{\mathbf{r}} = \mathbf{r}/r$. Boldfaced $\mathbf{1}$ is a unit matrix, and $\hat{\mathbf{r}}\hat{\mathbf{r}}$ is a dyadic (or tensor) multiplication of two unit vectors $\hat{\mathbf{r}}$. The incident electric field $\mathbf{E}_0(\mathbf{x})$ is

$$\mathbf{E}_0(x) = E_0\hat{\mathbf{e}}e^{ik\hat{\mathbf{k}}\cdot\mathbf{x}} \tag{3}$$

where $\hat{\mathbf{e}}$ is a unit vector specifying the wave's polarization, E_0 is the intensity of incident wave, $\hat{\mathbf{k}}$ is a unit vector defining the wave propagation, $k = 2\pi/\lambda$, and λ is wavelength. We now seek a solution of this integral equation to obtain the electric field and all the relevant scattering properties follow from this solution. Unfortunately, the integral (Fredholm) equation (1) is *not* easily solvable although it is amenable to a variety of approximations commonly used in scattering problems. In fact the approximate methods such as the Rayleigh approximation (also known as the Rayleigh-Gans-Debye (RGD), the Rayleigh-Gans-Rocard or the Kirchoff or the first Born approximation), the second and higher Born approximations, Anomalous Diffraction Theory (ADT) also known as High Energy Approximation (HEA) or the equivalent WKB method, the Discrete Dipole Approximation (DDA) and the Extended Boundary Method can all be derived directly from (1) (Saxon, 1955; Flatau and Stephens, 1988b).

4. Discrete Dipole Approximation

A useful and general way to solve (1) is to discretize the integral term thus reducing the integral equation to a linear system of equations. In the DDA approximation one assumes that each volume element may be replaced by a point dipole, whose (tensor) polarizability is related to the volume of the element and the dielectric tensor using the Clausius-Mossotti relations, corrected for the effects of radiative reaction. Each of the dipoles acquires a (time-dependent) polarization in response to the electric field at the position of the dipole, which includes contributions from all of the other dipoles plus the incident wave. This is the approach of the DDA as originally formulated by deVoe (1964) and Purcell and Pennypacker (1973). Consider our hexagonal crystal in this instance divided into

N discrete domains of volume v_j (Fig. 2) centered around point $\mathbf{x}_j$, where $j = 1, \ldots, N$. The volume of such an elementary domain is

$$v_j = \frac{V}{N} \tag{4}$$

where V is the volume of the particle, and N is the number of domains. Thus we are able to form a set of $3N$ equations from (1) since there are three components of the $\mathbf{E}$ field at each $\mathbf{x}_i$. The resulting equation set can then be represented in the form

$$\mathcal{A}\mathcal{P} = \mathcal{E}_0 \tag{5}$$

where P is the 3N-dimensional vector whose elements are the dipole moments of the N dipoles. For further details of the matrix structure and computational solution procedures the interested reader can consult the recent work of Draine (1988). The electric field everywhere in the three-dimensional space is given in terms of the structure matrix $\mathcal{A}$ which depends only on *particle's shape, refractive index and incident wavelength* but is independent of the direction and polarization of the incident wave $\mathbf{E}_0(\mathbf{x})$. Once $\mathcal{P}$ is determined then single scattering properties of the particle can be derived from the relationships reported by Draine (1988).

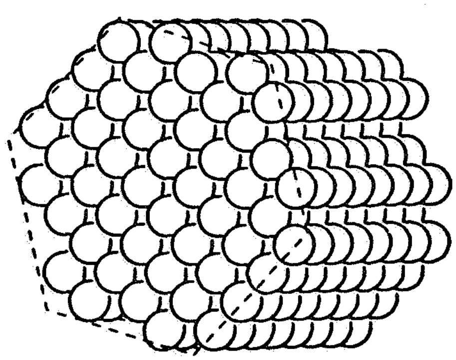

Fig. 2 *Hexagonal discrete dipole arrays with $N = 384$. Higher resolution was actually used, see text for further comments.*

The DDA method has been applied to calculate the scattering properties of small hexagonal ice crystals. Figure 2 presented the discrete dipole array for $N = 384$ dipoles but for the calculations reported in this paper actually used 2208 dipoles. The wavelength of $\lambda = 3.8\mu m$ and the corresponding value for the refractive index of ice $m = 1.38 + i0.0067$ was employed as was $\lambda = 10.8\mu m$ with a corresponding value $m = 1.089 + i0.182$. The wavelengths represent near infrared and infrared regions with small and relatively large absorption, respectively and correspond to central wavelengths of the AVHRR imager. The $10.8\mu m$ wavelength is also a relevant wavelength for application to CO_2 lidar studies.

The scattered intensity is presented in Fig. 3 as a function of scattering angle for two scattering planes, one perpendicular to $\mathbf{E}_0$ and the other parallel to $\mathbf{E}_0$.

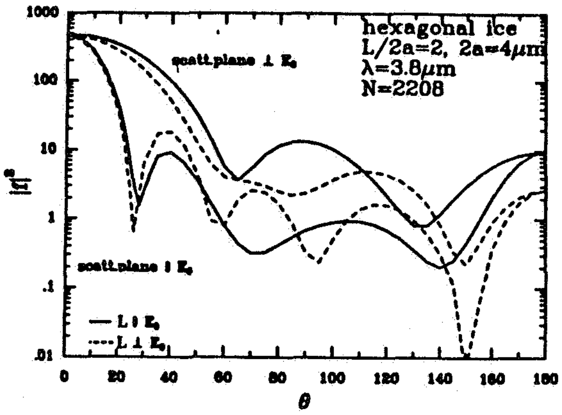

Fig. 3 *Intensities for hexagonal ice for an incident wave perpendicular to the crystal (average) and $\lambda = 3.8\mu m$. Results for two scattering planes are presented. Crystal length $L = 8\mu m$, crystal radius $a = 2\mu m$. $N = 2208$ discrete dipoles were used.*

The incident direction was taken to be normal to the L-axis of the hexagon, the length of the crystal used in the calculations is specified by L, and the aspect ratio is defined as $p = L/2a$ where $2a$ is the width of the crystal. Results are shown for two cases: incident electric field parallel to, and perpendicular to, the L-axis of the hexagon. Because the hexagon is not rotationally symmetric, the scattering problem depends upon the orientation of the hexagon. Two cases have been considered: (1) with the hexagon oriented so that the $\mathbf{k}$ vector is normal to one of the 6 rectangular faces, and (2) with the hexagon rotated by 30 degrees, so that the $\mathbf{k}$ vector is parallel to a line connecting a vertex to the center of the hexagon. (Each of these two cases has reflection symmetry which greatly reduces the amount of computing required to obtain a solution). The scattering intensities shown in Figures 3 and 4 are the averages of the scattering intensities for the above two cases.

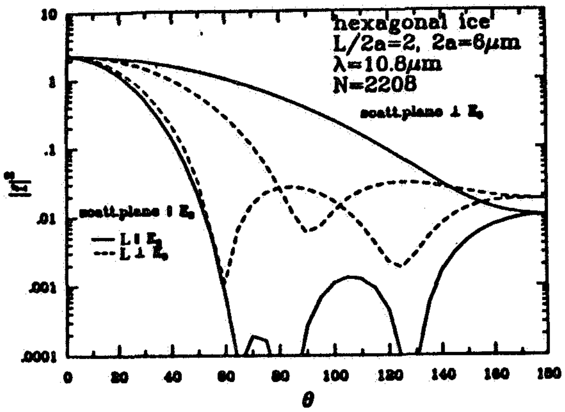

Fig. 4 *Same as Fig. 3 but for $\lambda = 10.8\mu m$. Crystal length $L = 8\mu m$, crystal radius $a = 2\mu m$.*

Figure 5 shows the results of the Mie calculation for a sphere with a volume equal to that of the hexagonal crystal. The intensities $|f|_{\parallel}^2$ and $|f|_{\perp}^2$ are presented here as a function of scattering angle and

$$|f|^2 = k^2 \frac{dC_{sca}}{d\Omega}. \tag{6}$$

(see e.g. Bohren and Huffman, 1983). There are several features worthy of mention in comparing between Figs. 3, 4 and 5. For example the backscatter linear polarization, defined as

$$\delta(\theta = 180) = \frac{|f|_{\perp}^2(\theta = 180) - |f|_{\parallel}^2(\theta = 180)}{|f|_{\perp}^2(\theta = 180) + |f|_{\parallel}^2(\theta = 180)} \tag{7}$$

is non-vanishing in case of hexagonals as compared to a zero depolarization for spheres. This is a well known characteristic of scattering by non-spherical particles but the quantitative relationship between δ and particle shape has never been convincingly established. The first minimum in intensity doesn't correspond to the Mie case, thus indicating that care has to be taken when interpreting results from the forward scattering PMS probes. This again is well established experimentally fact but its theoretical confirmation has to date been scarce. It seems that the extinction can be modelled, as it usually is, using a sphere of equivalent volume or surface, and we plan to perform more detailed calculations for the angularly averaged case.

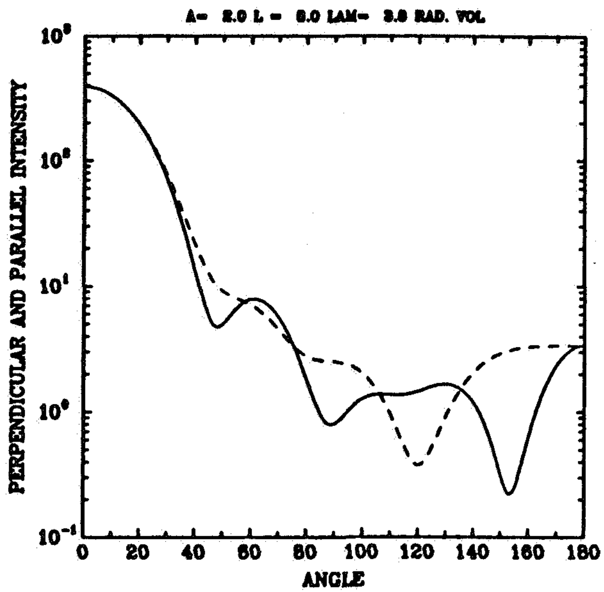

Fig. 5 *Mie results for equivalent volume spheres $r = 3.41\mu m$, and $\lambda = 3.8\mu m$.*

5. Anomalous Diffraction Theory

The anomalous diffraction theory (ADT) belongs to the broad class of approximations (together with the Rayleigh-Gans-Debye or Born expansions for example) in which one *makes some assumption about* the electric field under the integral of (1). This was noticed by Saxon (1955) and derived independently by van de Hulst (1957) on the basis of geometrical optics and diffraction. In the present context one assumes that the electric field inside the particle is given by

$$\mathbf{E}(\mathbf{x}) = E_0 \hat{\mathbf{e}} \exp\left[ik\hat{\mathbf{k}} \cdot (\mathbf{b} + \hat{\mathbf{e}}_z z) - \chi(\mathbf{b}, z)\right] \tag{8}$$

where $\chi(\mathbf{b}, z)$ corresponds to the phase change due to the changed refractive index inside the particle. The impact vector $\mathbf{b}$ is perpendicular to the z axis (see Fig. 6). The explicit formulation of $\chi(\mathbf{b}, z)$ and relation of ADT to other theories such as High Energy Approximation and DDA is contained in Flatau and Stephens (1988). The anomalous diffraction theory (ADT) (Stephens, 1984) holds for particles with a refractive index close to unity $(m - 1) \ll 1$ and for a particle with a size to wavelength ratio $x \gg 1$. Since the index of refraction is close to 1, the problem of *total* extinction in the ADT theory reduces to calculations of the interference between the almost straight transmission and the light diffracted according to Huygens' principle.

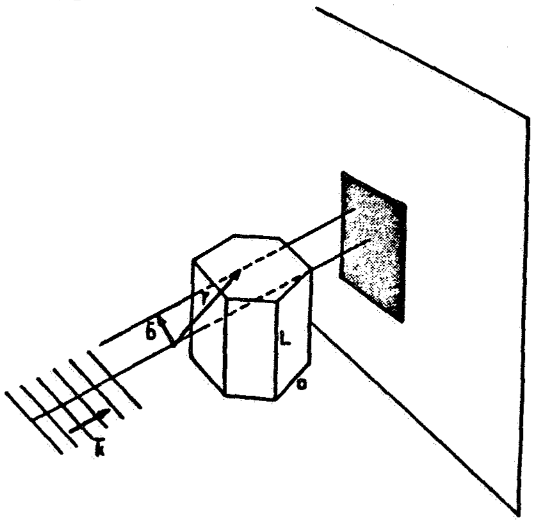

Fig. 6 *Geometry for Anomalous Diffraction Theory calculations.* **b** *is an impact parameter,* **r** *the position vector,* **k** *the direction of plane wave. The shadow area is in the far field and only forward scattering is considered here.*

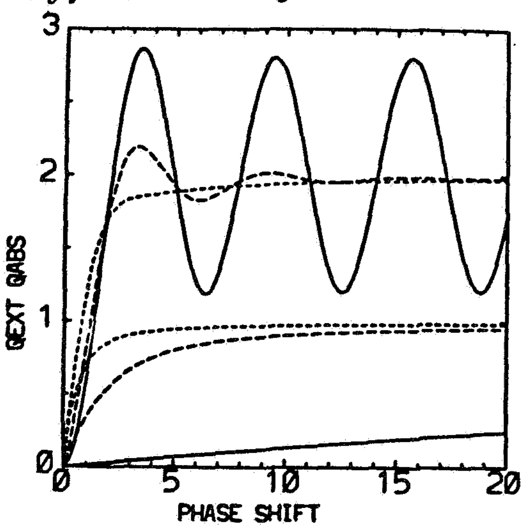

Fig. 7 *Extinction efficiency (converging or oscillating around 2 for large phase shift values) and absorption efficiency for hexagonal ice crystals for 3 different values of complex refractive index as a function of phase shift.*

Thus, in the anomalous diffraction approximation, the forward scattering amplitude $S(0)$ is given by

$$S(\theta = 0) = \frac{k^2}{2\pi} \int_A \left(1 - e^{-i\phi^*}\right) dA \qquad (9)$$

where $\phi^* = kd(m-1)$, d is the particle thickness, and m is the complex refraction: $m = n - in'$. The quantity ϕ^* is the complex phase shift of light passing through the particle relative to that passing around it. The kdn' term contributes to absorptive attenuation.

The extinction and absorption coefficients are defined as

$$C_{ext} = \frac{2}{A} Re \int_A \left(1 - e^{-i\phi^*}\right) dA \qquad (10)$$

and

$$C_{abs} = \frac{1}{A} \int_A \left(1 - e^{-2kdn'}\right) dA \qquad (11)$$

and the single scattering albedo is

$$\omega = \frac{C_{ext} - C_{abs}}{C_{ext}}. \qquad (12)$$

Therefore application of the ADT requires the relatively straight forward determination of the path length through the particle and evaluation of integrals for C_{sca} and C_{abs}. Notice that (8) is more general because it provides, in principle, the full phase function. Calculations of C_{ext}, C_{abs}, and ω for hexagonal crystals are presented in Figs. 7 and 8 using this approximation for the geometry depicted in Fig. 6. Full details of the method are planned in a forth coming paper and we also plan to compare these results, including phase functions, with solutions obtained from geometric optics and DDA.

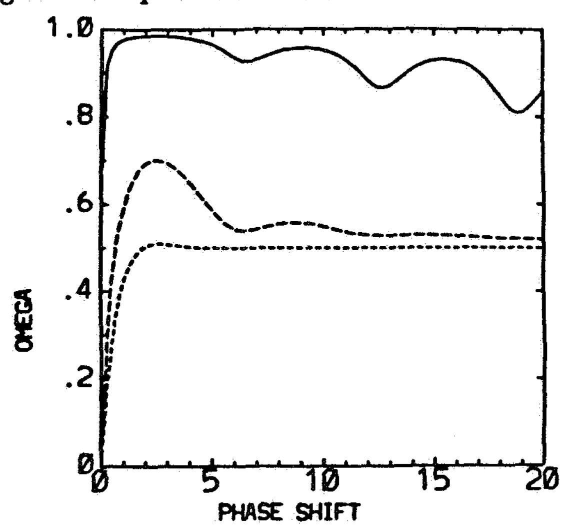

Fig. 8 *Single scattering albedo for hexagonal ice crystal in ADT approximation for 3 different values of complex refractive index.*

6. Summary

This paper reports on new calculations of the scattering of radiation by hexagonal ice crystals. Results are presented for small crystals which are not only the first of their type but also employ methods, to our knowledge, not previously used in atmospheric scattering problems. Scattering properties of large hexagonal crystals were also modelled using more approximate theories. While the results presented in this paper apply only to hexagonal crystals, the methods are general and particles of other geometries will be considered in further studies.

The work reported in this paper is preliminary and we plan to use the microphysic data collected during FIRE into these calculations to obtain the optical properties needed in the radiative transfer simulations of the cloud flux measurements.

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