JP3.2

TESTING OF THE MODIFIED ANOMALOUS DIFFRACTION APPROXIMATION WITH T-MATRIX CALCULATIONS FOR HEXAGONAL COLUMNS

David L. Mitchell[1] and Anthony J. Baran[2]
1. Desert Research Institute, Reno, Nevada
2. U.K. Met. Office, Bracknell, U.K.

1. INTRODUCTION

In the treatment of ice cloud radiative properties, two approaches have been taken: (1) parameterization of exact results from electrodynamic scattering theory in terms of bulk microphysical properties (e.g. IWC and effective size) and (2) parameterization of electrodynamic scattering theory itself in terms of explicit microphysical properties (e.g. size distribution parameters, ice crystal mass and area relationships). The strength of the first approach lies in the single particle calculations, while the strength of the second approach lies in the explicit coupling of microphysical and radiative properties. This study tests the weakest aspect of the second approach: the accuracy of ice crystal single scattering properties.

This second approach we can call the modified anomalous diffraction approximation, or modified ADA, as described in Mitchell (2000; 2002). This approach uses a specific form of the ADA first proposed by Bryant and Latimer (1969), and later developed in Mitchell and Arnott (1994) and in Mitchell et al. (1996). As pointed out by Sun and Fu (2001), this form differs from the ADA developed by van de Hulst (1957) in that instead of performing an integration of ray-paths through the particle, a single ray-path is used and is defined as the particle volume V corresponding to the bulk density of ice (0.92 g cm^{-3}) divided by the particle's projected area P (assuming either random or some preferred orientation). This quantity V/P is referred to as the effective photon path, and results in a much simplified form of ADA, amenable to analytical solutions for the size distribution absorption and extinction coefficients, β_{abs} and β_{ext}, for any particle shape. Perhaps due to this departure from standard ADA, this simplified ADA is not mentioned in some recent books on light scattering by non-spherical particles (e.g. Mishchenko et al. 2000).

Corresponding author address: David L. Mitchell, DRI, Division of Atmospheric Sciences, 2215 Raggio Pkwy, Reno, NV 89512-1095; e-mail: mitch@dri.edu

It is argued here that this simplification not only has computational advantages, but by embracing the V/P concept, the formulation is more accurate than the standard ADA, as discussed below.

The scattering/absorption processes of internal reflection and refraction, and photon tunneling, are neglected in the ADA, but have recently been parameterized into the simplified ADA for both spherical (Mitchell et al. 2000) and non-spherical (Mitchell 2002) cloud particles. Photon tunneling accounts for radiation beyond the physical cross-section of a particle that is either absorbed or scattered outside the forward diffraction peak. This new analytical form of ADA will henceforth be referred to as modified ADA, and was found to yield agreement with Mie theory for water and ice spheres within 10%. Sun and Fu (2001) have shown that the V/P ADA may differ from the standard ADA by up to 100% for extinction efficiencies (Q_{ext}) using spheres, cylinders and hexagonal columns. If the V/P ADA had similar errors, these large errors would be evident in Q_{ext} predicted by modified ADA. But as seen in Fig. 8 of Mitchell (2000), the modified ADA Q_{ext} exhibits little error relative to Mie theory, even when absorption is low. Moreover, it was demonstrated in Mitchell (2002) that the reason that the effective radius r_{eff} (as defined for water clouds) is successful when used in Mie theory in accurately producing the size distribution (SD) β_{abs} for water clouds is because r_{eff} is essentially V/P for a SD. That is, the physical basis behind r_{eff} is that the absorption properties of a monomodal SD can be accurately described by the V/P of the entire SD. For instance, note that an alternate quantity for r_{eff} is effective diameter D_{eff} (D_{eff} = 2 r_{eff}), where D_{eff} is defined as

$$D_{eff} = \frac{3}{2}\,\frac{WC}{\rho\, P_t} \qquad (1)$$

where WC = liquid or ice water content (e.g. g m^{-3}), ρ = bulk density for water or ice (e.g. g cm^{-3}), and P_t = SD projected area (e.g. cm^2 m^{-3}). The second term in (1) is V/P for the SD, while the prefactor 3/2 is due to the fact that for a sphere, V/P = 2/3 D where D is diameter (e.g. $V = \pi D^3/6$, $P = \pi D^2/4$). Since D_{eff} refers to the diameter of a sphere, the prefactor is needed. The accuracy of D_{eff} when used in Mie theory to describe β_{abs} lends strong support to the idea that the effective photon path is the appropriate distance for describing the radiative properties of both individual particles and size distributions. [However, the utility of D_{eff} is impaired when SDs become bimodal, as found in ice clouds, making it necessary to deal with the actual SD as described in Mitchell (2002)]. For these reasons, it is argued that the V/P version of ADA provides greater accuracy than the original ADA

1.1 *Disadvantages of modified ADA*

The main disadvantage of modified ADA is that it is not based on an exact electrodynamic solution for a specific particle shape, such as T-matrix (e.g. Mishchenko et al. 1996; Havemann and Baran 2001) or the finite difference time domain method (FDTD; Yang and Liou 1995; 1996). Rather, it is based on the principle of an effective photon path d_e, whereby the scattering/absorption processes are parameterized based on ice particle d_e. Mie theory was used to develop and test the parameterizations for the processes of internal reflection/refraction and photon tunneling.

Since external reflection was not explicitly parameterized, the contribution to absorption from geometric optics may be overestimated somewhat, where V/P ADA represents the geometric optics contribution. Note external reflection reduces absorption. For extinction, external reflection is implicitly accounted for by ADA. However, errors between modified ADA and Mie theory are no worse than 10% for size spectra found in water clouds and cirrus (Mitchell 2000; Ivanova et al. 2001; Mitchell 2002), suggesting that the parameterization of the photon tunneling process may have compensated for potential absorption errors resulting from the absence of external reflection. Nonetheless, the Baran and Havemann (1999) tunneling parameterization yields results very similar to the modified ADA tunneling parameterization (Mitchell et al. 2001). As size parameter x increases beyond 30, the absence of external reflection is apparent as $\overline{Q}_{abs}$ for Mie theory drops below 1.0 for strong absorption, while the modified ADA $\overline{Q}_{abs}$ asymptotes to 1.0. Note $\overline{Q}_{abs}$ is defined as the ratio of the SD absorption coefficient β_{abs} to SD projected area P_t, or $\overline{Q}_{abs} = \beta_{abs}/P_t$. This failure of the modified ADA $\overline{Q}_{abs}$ to drop below 1.0 may cause errors up to 15% for $x > 150$, but such errors are generally on the order of 7% for refractive indices associated with water and ice. An example of relatively large external absorption error is shown in Fig. 7 of Mitchell (2000). Since external reflection errors appear to be trivial for SD characteristic of cirrus clouds (due to $x < 60$), this process was not included when formulating the modified ADA.

1.2 *Advantages of modified ADA*

Modified ADA has the following advantages:

• It is analytical and extremely computationally efficient relative to more "first principle" methods.

• Since $d_e = V/P = m/\rho_i P$ where m = particle mass and ρ_i = 0.92 g cm^{-3} (density of solid ice), any particle shape can be used provided the power laws giving its projected area- and mass-dimensional relation are known.

• The properties of the SD and the ice particle shapes are present in the solutions for β_{abs} and β_{ext}, which were derived from the integral definitions of β_{abs} and β_{ext}. This makes modified ADA a useful tool for exploring the interrelationships between radiation and cloud microphysics, as the SD and particle properties are easily altered. For example, modified ADA has recently been used to evaluate the presence of high concentrations of small (D < 100 μm) ice crystals in cirrus, and to test SD parameterizations (Mitchell et al. 2002, these postprints).

• The main physical processes were parameterized and thus can be isolated to better understand their role in the absorption/scattering process.

• The contribution of photon tunneling to absorption and extinction depends on particle morphology (Baran and Havemann 1999). Ice particles in cirrus generally have complex, irregular shapes (e.g. Korolov et al. 1999; 2000). Thus it is likely that the idealized crystal shapes used in electrodyamic realizations of absorption/scattering are unrealistic, raising the possibility that predicted tunneling contributions to absorption may not apply to natural cirrus. The contribution of tunneling in modified ADA depends on an arbitrary tunneling factor, T_f, that varies between 0 (no tunneling) and 1.0 (maximum tunneling corresponding to spheres and Mie theory). Recent work (Mitchell et al. 2002, these postprints) indicates that T_f may be retrieved via ground based or satellite measurements of thermal radiances. If T_f

can be characterized for cirrus, then modified ADA should be able to accurately predict longwave radiative properties for cirrus.

- As shown below, modified ADA agrees relatively well with T-matrix for the same ice crystal type and SD. The same is true for comparisons with laboratory measurements of $\overline{Q}_{ext}$ (Mitchell et al. 2001). Thus the errors associated with modified ADA appear small relative to other factors affecting cloud-radiation interactions, such as cloud microphysics.

2. MIXTURES OF ICE PARTICLE SHAPE

Another advantage of modified ADA is that any cloud composition of ice particle shape may be assumed. The simplest approach is to determine mass-dimensional (m-D) and projected area-dimensional (P-D) relationships for any given mixture of ice particle shape. These relationships have the form:

$$m = \alpha D^{\beta}, \tag{2}$$

$$P = \gamma D^{\sigma}, \tag{3}$$

where m is mass, P is projected area, and D is particle maximum dimension. The constants corresponding to these power laws are used in the solutions for β_{abs} and β_{ext}, so it is best to determine single values for α, β, γ and σ when dealing with mixtures of particle shapes. This simplifies the calculations for β_{abs} and β_{ext} considerably.

The m-D and P-D relationships often change for a given crystal type at D = 100 μm. Therefore a set of mass or area constants is determined for D < 100 μm and for D > 100 μm, which apply to a given mixture of ice particle shapes. Since it is a given that m and P are related to D via a power law, m and P can be determined at selected D values and used to define a line in log-log space. For example, the D values used for a given shape, giving one or two line equations, may be 10 μm, 100 μm, and 1000 μm. For a given D value and mixture of shapes, the representative ice particle mass may be given as

$$m_{mix} = m_{ros}\,(F_{ros}/F_t) + m_{pp}\,(F_{pp}/F_t) + m_p\,(F_p/F_t) + m_c\,(F_c/F_t) \tag{4}$$

where ros, pp, p and c refer to rosettes, planar polycrystals, plates and columns, respectively, F refers to the fraction or percentage of a given shape, and F_t is the total of these:

$$F_t = F_{ros} + F_{pp} + F_p + F_c\,. \tag{5}$$

It is necessary to assume here that a given F applies equally over all particle sizes in either the small particle mode (D < 100 μm) or large particle mode of a bimodal SD. For a given crystal size and shape, m and P can be obtained from m-D and P-D relations in the literature (e.g. Mitchell et al. 1996; Mitchell 1996). In this way, m_{mix} may be determined for the three D values noted above. If solving for the small ice particle mode, D_1 = 10 μm, D_2 = 100 μm, and

$$\beta_{mix} = \frac{\ln m_{mix,2} - \ln m_{mix,1}}{\ln D_2 - \ln D_1}\,, \tag{6}$$

$$\alpha_{mix} = \exp(\ln m_{mix,2} - \beta_{mix} \ln D_2)\,. \tag{7}$$

Equations analogous to (6) and (7) can be written for D > 100 μm (i.e. large particle mode). The procedure for determining γ_{mix} and σ_{mix} regarding the P-D power laws is analogous to this procedure.

3. TESTING OF MODIFIED ADA

Modified ADA has already been tested with regards to SD extinction efficiencies ($\overline{Q}_{ext}$) measured during a laboratory experiment, where $\overline{Q}_{ext} = \beta_{ext}/P_t$ (Mitchell et al. 2001). The ice particle SD was measured in a cloud chamber by two instruments, the Forward Scattering Spectrometer Probe (FSSP) and the Cloudscope, which video records particles impacted at high collection efficiency. Good agreement was found between SDs measured by the two instruments, in spite of very different operating principles. The SD and aspect ratios of the hexagonal columns comprising the ice cloud were used in modified ADA and in T-matrix calculations to predict $\overline{Q}_{ext}$. This new implementation of T-matrix incorporates the exact geometry of hexagonal columns, without approximating them as spheroids or circular cylinders (Havemann and Baran 2001). The $\overline{Q}_{ext}$ predicted by the modified ADA and T-matrix were compared between 8.3-12 μm wavelength, while $\overline{Q}_{ext}$ from modified ADA was compared against measured values of $\overline{Q}_{ext}$ from 2-14 μm wavelength. The $\overline{Q}_{ext}$ was measured via Fourier transform infrared spectroscopy (FTIR) inside the ice cloud. Since D_{eff} for the SD was only 14 μm, the low size parameters ($x = \pi D_{eff}/\lambda$) resulted in a wide variation in $\overline{Q}_{ext}$ values, posing a challenging test of theory. Using a photon tunneling factor around 0.6, the mean difference between the $\overline{Q}_{ext}$ predicted from modified ADA and the measured $\overline{Q}_{ext}$ was 3%, with similar agreement obtained for the T-matrix calculations.

Since modified ADA has already been tested for extinction in the above study, the new aspect in this study is absorption. The excellent agreement between T-matrix and the $\overline{Q}_{ext}$ measurements noted above provides confidence that $\overline{Q}_{abs}$ ($\overline{Q}_{abs} = \beta_{abs}/P_t$) predicted by T-matrix can be used to test the accuracy of $\overline{Q}_{abs}$ predicted by modified ADA. In addition, $\overline{Q}_{ext}$ from modified ADA and T-matrix will be compared over a greater wavelength range than in Mitchell et al. (2001). All calculations shown here are based on the SD measured by the Cloudscope in Mitchell et al. (2001).

Modified ADA is compared with this new implementation of T-matrix for $\overline{Q}_{ext}$ in Fig. 1 and for $\overline{Q}_{abs}$ in Fig. 2, based on a tunneling factor of 0.6 (consistent with Mitchell et al. 2001). The measured $\overline{Q}_{ext}$ are shown by the solid curve in Fig. 1, with measured $\overline{Q}_{ext}$ excluded from regions where water vapor or CO_2 absorption was significant (gaps in Fig. 1). The lower curve in Fig. 1 indicates the contribution from photon tunneling. In Mitchell et al. (2001), the measurements indicated that edge effects (i.e. tunneling resulting in surface waves) did not contribute to $\overline{Q}_{ext}$, and therefore edge effects were "turned off" for the modified ADA predictions here. Where wavelength resolution was low, T-matrix calculations are shown by circles in Fig. 1 and Fig. 2 (instead of the long-dashed curve). In Fig. 2, T-matrix is shown by the solid curve, modified ADA by the short-dashed curve, the photon tunneling contribution is shown by the long-dashed curve, and the contribution of internal reflection/refraction to absorption is indicated by the dotted curve (lowest in figure). Again, T-matrix calculations are indicated by circles where wavelength resolution is low.

Percent errors for modified ADA, relative to T-matrix and corresponding to Figs. 1 and 2, are shown in Fig. 3 and 4. These comparisons can be summarized as follows. The mean difference between the Q_{ext} predicted from modified ADA and the measured Q_{ext} was 3.5%, with the same agreement (3.5%) obtained for T-matrix. The mean modified ADA error for absorption relative to T-matrix was 5.0%, while the maximum error was 15%. Comparing the modified ADA Q_{ext} with T-matrix, the mean error relative to T-matrix was 4.1%, while the maximum error was 8.0%. The low size parameters used in these comparisons allow for wide variation in both $\overline{Q}_{ext}$ and $\overline{Q}_{abs}$, providing a rigorous test of modified ADA.

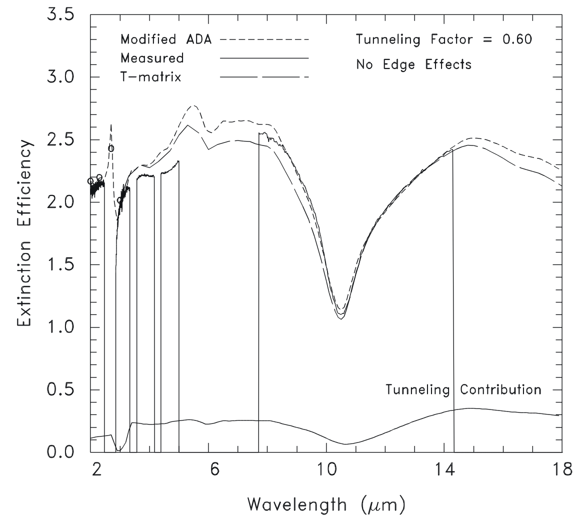

Figure 1. Comparison of modified ADA and T-matrix with measured Q_{ext}. Regions without data were contaminated by water vapor absorption.

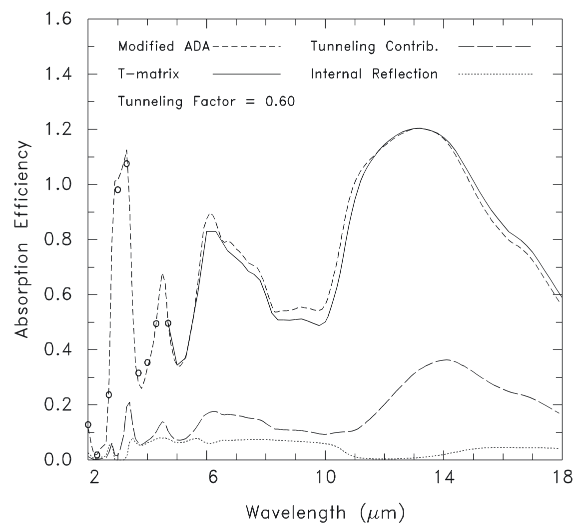

Figure 2. Comparison of modified ADA with T-matrix, using the same SD and tunneling factor as in Fig. 1.

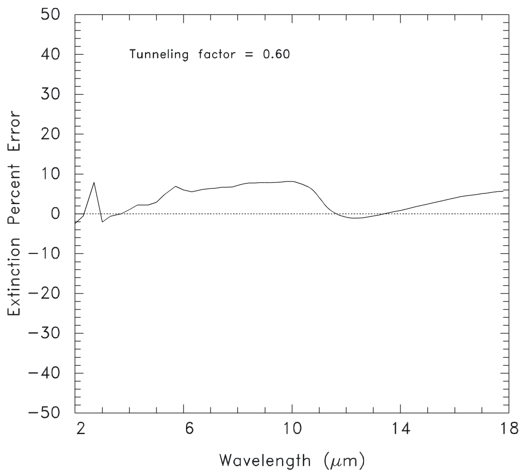

Figure 3. Modified ADA extinction error relative to T-matrix, corresponding to Fig. 1.

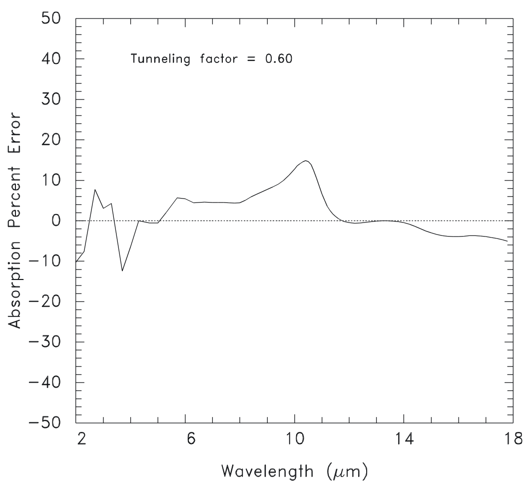

Figure 4. Modified ADA absorption error relative to T-matrix, corresponding to Fig. 2.

4. COMPARISON WITH FU SCHEME

While not a test of accuracy, it is of interest to compare modified ADA with the ice cloud radiation scheme of Fu (1996) and Fu et al. (1998) for terrestrial radiation, in the same manner as described in Mitchell (2002). The tropical bimodal SD parameterization of Mitchell et al. (2000) was used to compare schemes, with D_{eff} = 25.7 µm. This provided for a wide variation in $\overline{Q}_{abs}$ and $\overline{Q}_{ext}$ for a more meaningful comparison. The large mode mean maximum dimension was 74 µm. The tunneling factor was 0.60, corresponding to hexagonal columns (Mitchell et al. 2001), allowing for a direct comparison between schemes (note the Fu scheme implicitly assumes tunneling corresponding to hexagonal columns). The two schemes are compared in Figs. 5 and 6 for absorption and extinction, respectively.

The Fu et al. (1998) scheme terminates at λ = 100 µm. The disagreement at longer λ is likely due to differences in the SDs used to parameterize the Fu schemes and the tropical SD scheme used here, as discussed in Mitchell (2002). Since the λ resolution in the near infrared is crude regarding Fu (1996), comparisons in this region are not meaningful. But for λ between 3 and 45 µm, the agreement appears good. Percent differences between schemes for absorption were generally within 10% for these λ. One exception is the trough around λ = 4 µm (see Fig. 5), which was also pointed out in Mitchell (2002). It is not clear why this minimum is higher than the minimum at λ = 5 µm, since the imaginary refractive index is lower at λ = 4 µm than at 5 µm. For extinction, percent differences are within 10% for all but the longest λ. Overall, Fu scheme which utilizes the FDTD method and the modified ADA scheme compare favorably.

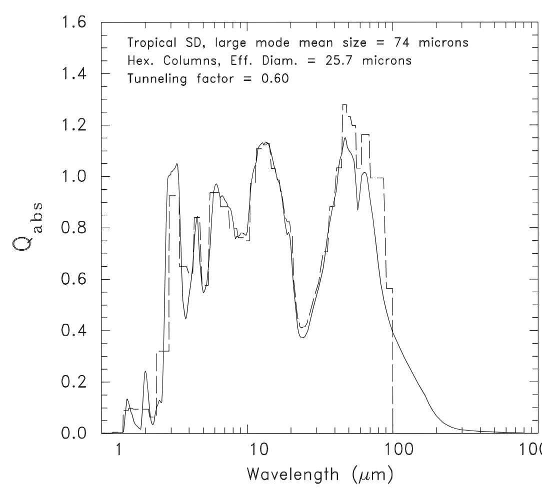

Figure 5. Comparison between the Fu schemes (dashed) and modified ADA for the conditions indicated regarding $\overline{Q}_{abs}$.

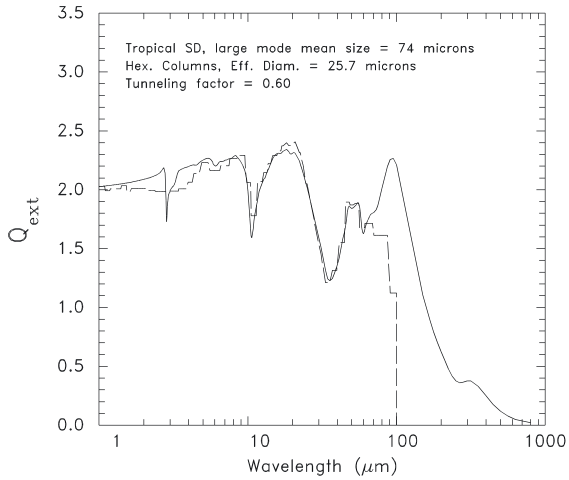

Figure 6. Comparison between the Fu schemes (dashed) and modified ADA (solid) for the conditions indicated, regarding $\overline{Q}_{ext}$.

REFERENCES

Baran, A.J., S. Havemann, 1999: Rapid computation of the optical properites of hexagonal columns using complex angular momentum theory. *JQRST*, **63**, 499-519.

Baran, A.J., S. Havemann, P.N. Francis, and P. Yang, 2001: A study of the absorption and extinction properties of hexagonal ice columns and plates in random and preferred orientation, using exact T-matrix theory and aircraft observations of cirrus. *JQSRT*, **70**, 505-518.

Bryant, F.D., and P. Latimer, 1969: Optical efficiencies of large particles of arbitrary shape and orientation. *J. Colloid and Interface Sci.*, **30**, 291-304.

Fu, Q., 1996: An accurate parameterization of the solar radiative properties of cirrus clouds for climate models. *J. Climate*, **9**, 2058-2082.

Fu, Q., P. Yang and W.B. Sun, 1998: An accurate parameterization of the infrared radiative properties of cirrus clouds for climate models. *J. Climate*, **11**, 2223-2237.

Havemann, S., and A.J. Baran, 2001: Extension of T-matrix to scattering of electromagnetic plane waves by non-axisymmetric dielectric particles: Application to hexagonal cylinders. *JQSRT*, **70**, 139-158.

Ivanova, D., D.L. Mitchell, W.P. Arnott and M. Poellot, 2001: A GCM parameterization for bimodal size spectra and ice mass removal rates in mid-latitude cirrus clouds. *Atmos. Res.*, **59**, 89-113.

Korolev, A.V., G.A. Isaac and J. Hallett, 1999. Ice particle habits in Arctic clouds. *Geophys. Res. Lett.* **26**, 1299-1302.

Korolev, A.V., G.A. Isaac and J. Hallett, 2000. Ice particle habits in stratiform clouds. *Q.J.R. Meteorol. Soc.* **126**, 2873-2902.

Mishchenko, M.I., L.D. Travis, and D.W. Mackowski, 1996: T-matrix computations of light scattering by nonspherical particles: A review. *JQSRT*, **55**, 535-575.

Mishchenko, M.I., J.W. Hovenier, and L.D. Travis, 2000: Light Scattering by Nonspherical Particles. Academic Press, 690 pp.

Mitchell, D.L., and W.P. Arnott, 1994: A model predicting the evolution of ice particle size spectra and radiative properties of cirrus clouds. Part II: Dependence of absorption and extinction on ice crystal morphology. *J. Atmos. Sci.*, **51**, 817-832.

Mitchell, D.L., 1996: Use of mass- and area-dimensional power laws for determining precipitation particle terminal velocities. *J. Atmos. Sci.*, **53**, 1710-1723.

Mitchell, D.L., A. Macke, and Y. Liu, 1996: Modeling cirrus clouds. Part II: Treatment of radiative properties. *J. Atmos. Sci.*, **53**, 2967-2988.

Mitchell, D.L., D. Ivanova, A. Macke and G.M. McFarquhar, 2000: A GCM parameterization of bimodal size spectra for ice clouds. Proceedings of the 9th ARM Science Team Meeting, March 22-26, 1999, San Antonio Texas (http://www.arm.gov/docs/ documents/ technical/conference.html).

Mitchell, D.L., 2000: Parameterization of the Mie extinction and absorption coefficients for water clouds. *J. Atmos. Sci.*, **57**, 1311-1326.

Mitchell, D.L., W.P. Arnott, C. Schmitt, A.J. Baran, S. Havemann and Q. Fu, 2001: Contributions of photon tunneling to extinction in laboratory grown hexagonal columns. *JQSRT*, **70**, 761-776.

Mitchell, D.L., 2002: Effective diameter in radiation transfer: Definition, applications and limitations. *J. Atmos. Sci.*, **59**, 2330-2346.

Sun, W., and Q. Fu, 2001: Anomalous diffraction theory for randomly oriented nonspherical particles: a comparison between original and simplified solutions. *JQRST*, **70**, 737-747.

van de Hulst, H.C., 1981: *Light Scattering by Small Particles*. Dover, 470 pp.

Yang, P., and K.N. Liou, 1995: Light scattering by hexagonal ice crystals: comparison of finite-difference time domain and geometric optics models. *J. Opt. Soc. Am. A*, **12**, 162-176.

Yang, P., and K.N. Liou, 1996: Finite-difference time domain method for light scattering by small ice crystals in three-dimensional space. *J. Opt. Soc. Am. A*, **13**, 2072-2085.