

Testing of the Modified Anomalous Diffraction Approximation with T-Matrix Calculations for Hexagonal Columns

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Introduction

In the treatment of ice cloud radiative properties, two approaches have been taken: 1) parameterization of exact results from electro-dynamic scattering theory in terms of bulk microphysical properties (e.g., ice water content 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 second approach regarding the accuracy of ice crystal single scattering properties.

This second approach we can call the modified anomalous diffraction approximation, or modified anomalous diffraction approximation (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 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. 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 original 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 original 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 Figure 8 of Mitchell (2000), the modified ADA Q_{ext} for single particles exhibits little error relative to Mie theory, even when absorption is low. Contributions to Q_{ext} from processes not included in ADA are also shown in this figure, making it clear that modified ADA, which includes these processes, would exhibit even greater differences relative to the original ADA than V/P ADA does. 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} ($D_{\text{eff}} = 2 r_{\text{eff}}$), where D_{eff} is defined as

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

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., $\text{cm}^2 \text{m}^{-3}$). 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 this reason, and because Q_{ext} from modified ADA appears more accurate than Q_{ext} from the original ADA, it is argued that the V/P version of ADA provides for greater accuracy than the original ADA, at least for Q_{ext} .

Disadvantages of Modified ADA

The main criticism 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 the process of external reflection was not included in modified ADA for absorption, some justification for its omission appears warranted. The absence of this process may imply that the contribution to absorption from geometric optics may be overestimated somewhat, where V/P ADA plus internal reflection/refraction 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; 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, based on absorption contributions exceeding the geometric optics contribution, yields results very similar to the modified ADA tunneling parameterization (Mitchell et al. 2001). This suggests the tunneling estimates are reasonably accurate in modified ADA. As size parameter x increases beyond 30, the absence of external reflection is apparent as Q_{abs} for Mie theory drops below 1.0 from strong absorption, while the modified ADA Q_{abs} asymptotes to 1.0. Note Q_{abs} is defined as the ratio of the SD absorption coefficient β_{abs} to SD projected area P_t , or $Q_{\text{abs}} = \beta_{\text{abs}}/P_t$. This failure of the modified ADA 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 Figure 7 of Mitchell (2000). Since external reflection errors appear to be trivial for SD characteristic of cirrus clouds (due to $x < 60$; e.g., Ivanova et al. 2001), this process was not included when formulating the modified ADA.

Advantages of Modified ADA

Modified ADA has the following advantages:

- As shown in the next section, 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 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.
- There is no one exact electrodynamic theory that applies to all wavelengths over the range of ice particle sizes found in cirrus clouds, nor does an exact theory exist that can treat any ice particle shape. While not an exact solution, modified ADA does not suffer from these limitations.
- 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 $\rho_i = 0.92 \text{ g cm}^{-3}$ (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 ($D < 100 \mu\text{m}$) ice crystals in cirrus and to test SD parameterizations (Mitchell et al. 2002, these proceedings).

- The main physical processes were parameterized and 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 electrodynamic 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 , which varies between 0 (no tunneling) and 1.0 (maximum tunneling corresponding to spheres and Mie theory). Recent work (Mitchell et al. 2002, these proceedings) 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.

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:

$$m = \alpha D^\beta, \quad (2)$$

$$P = y D^\alpha, \quad (3)$$

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 , y , 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 $D = 100 \mu\text{m}$. Therefore, a set of mass or area constants is determined for $D < 100 \mu\text{m}$ and for $D > 100 \mu\text{m}$, 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 $10 \mu\text{m}$, $100 \mu\text{m}$, and $1000 \mu\text{m}$. For a given D value and mixture of shapes, the representative ice particle mass m may be given as

$$m_{\text{mix}} = m_{\text{ros}} (F_{\text{ros}}/F_t) + m_{\text{pp}} (F_{\text{pp}}/F_t) + m_{\text{p}} (F_{\text{p}}/F_t) + m_{\text{c}} (F_{\text{c}}/F_t) \quad (4)$$

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:

$$F_t = F_{ros} + F_{pp} + F_p + F_c. \quad (5)$$

It is necessary to assume here that a given F applies equally over all particle sizes in either the small particle mode ($D < 100 \mu\text{m}$) 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; Heymsfield et al. 2002). In this way, m_{mix} may be determined for the three D values noted above. If solving for the small ice particle mode, $D_1 = 10 \mu\text{m}$, $D_2 = 100 \mu\text{m}$, and

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

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

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

Testing of Modified ADA

Modified ADA has already been tested with regard to SD extinction efficiencies (Q_{ext}) measured during a laboratory experiment, where $Q_{ext} = \beta_{ext}/P_t$ (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 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 Q_{ext} predicted by the modified ADA and T-matrix were compared between 8.3-12 μm wavelength, while Q_{ext} from modified ADA was compared against measured values of Q_{ext} from 2-14 μm wavelength. The 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 Q_{ext} values, posing a challenging test of theory. Using a photon-tunneling factor around 0.6, the mean difference between the Q_{ext} predicted from modified ADA and the measured 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 Q_{ext} measurements noted above provides confidence that Q_{abs} ($Q_{abs} = \beta_{abs}/P_t$) predicted by T-matrix can be used to test the accuracy of Q_{abs} predicted by modified ADA. In addition, 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 Q_{ext} in Figure 1 and for Q_{abs} in Figure 2, based on a tunneling factor of 0.6 (consistent with Mitchell et al. 2001). The measured Q_{ext} are shown by the solid curve in Figure 1, with measured Q_{ext} excluded from regions where water vapor or CO_2 absorption was significant (gaps in Figure 1). The lower curve in Figure 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 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 Figures 1 and 2 (instead of the long-dashed curve). In Figure 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 Figures 1 and 2, are shown in Figures 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

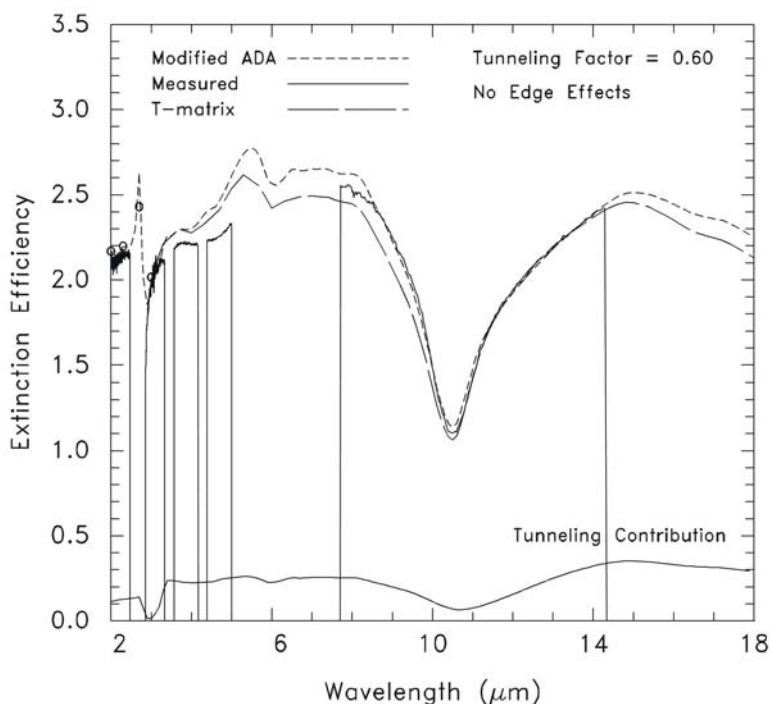


Figure 1. Comparison of modified ADA and T-matrix with measured Q_{ext} regions without data were contaminated by water vapor absorption.

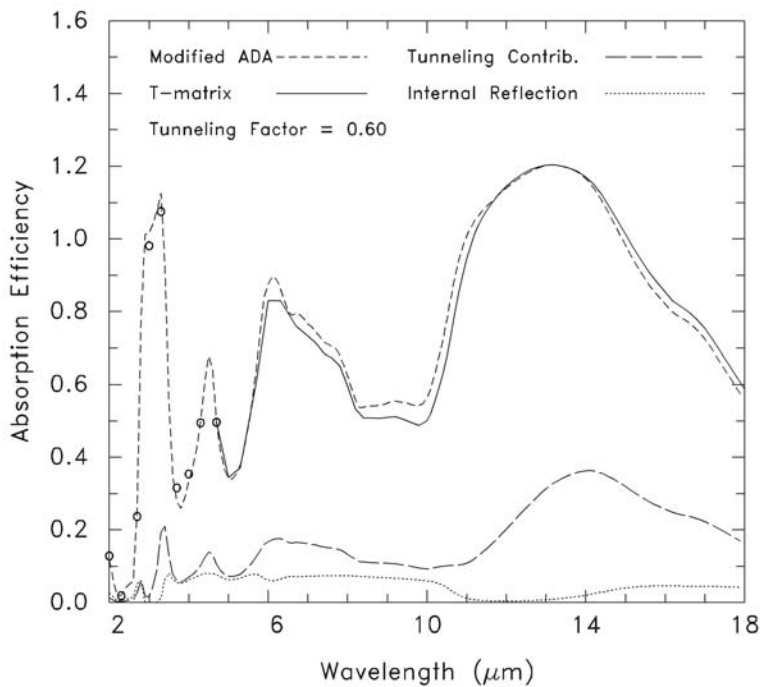


Figure 2. Comparison of modified ADA with T-matrix, using the same SD and tunneling factor as in Figure 1.

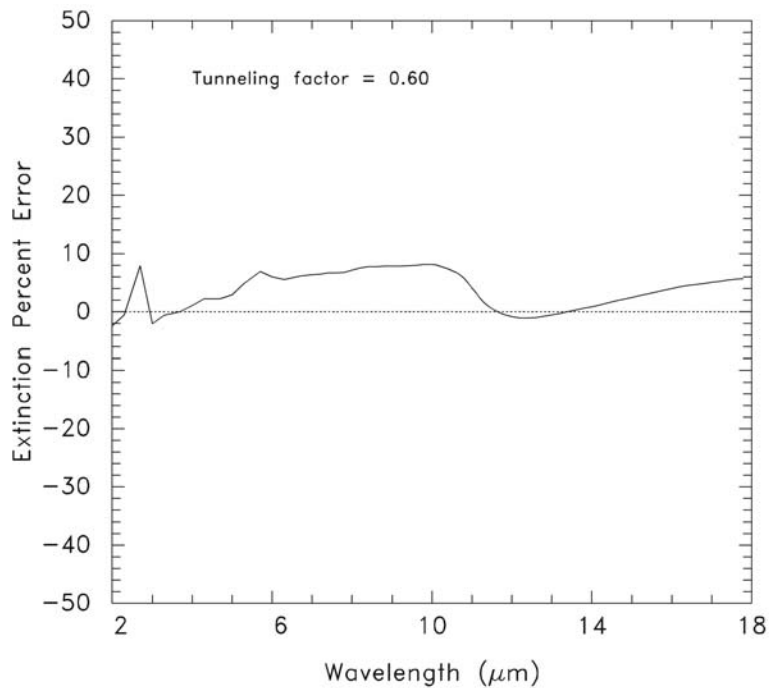


Figure 3. Modified ADA extinction error relative to T-matrix, corresponding to Figure 1.

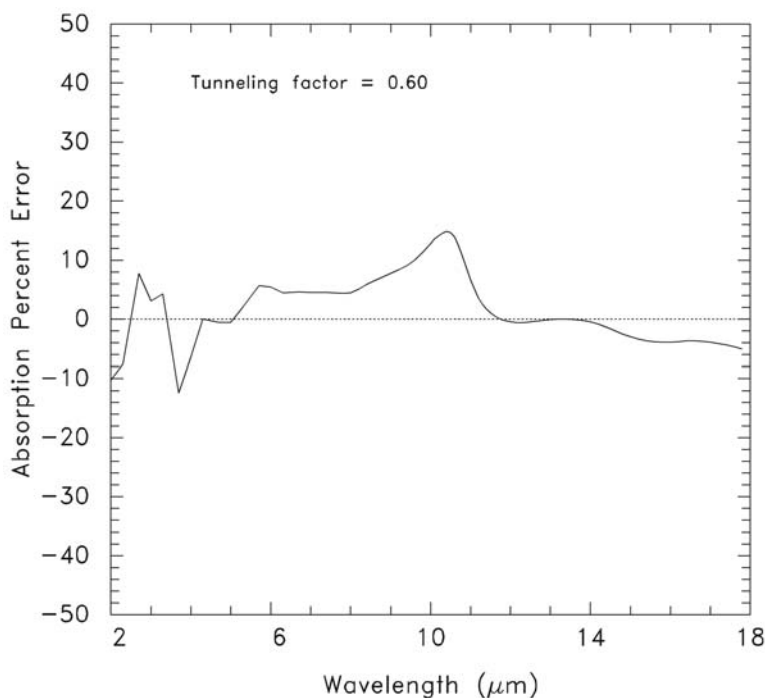


Figure 4. Modified ADA absorption error relative to T-matrix, corresponding to Figure 2.

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 Q_{ext} and Q_{abs} , providing a rigorous test of modified ADA.

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 $D_{\text{eff}} = 25.7 \mu\text{m}$. This provided for a wide variation in Q_{abs} and Q_{ext} for a more meaningful comparison. The large mode mean maximum dimension was $74 \mu\text{m}$. 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 Figures 5 and 6 for absorption and extinction, respectively.

The Fu et al. (1998) scheme terminates at $\lambda = 100 \mu\text{m}$. 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 for Q_{abs} . But for λ between 3 and $45 \mu\text{m}$, the agreement appears good. Percent differences between schemes for absorption were generally within 10% for these λ . The exception is the trough around $\lambda = 4 \mu\text{m}$ (see Figure 5), which was also addressed in

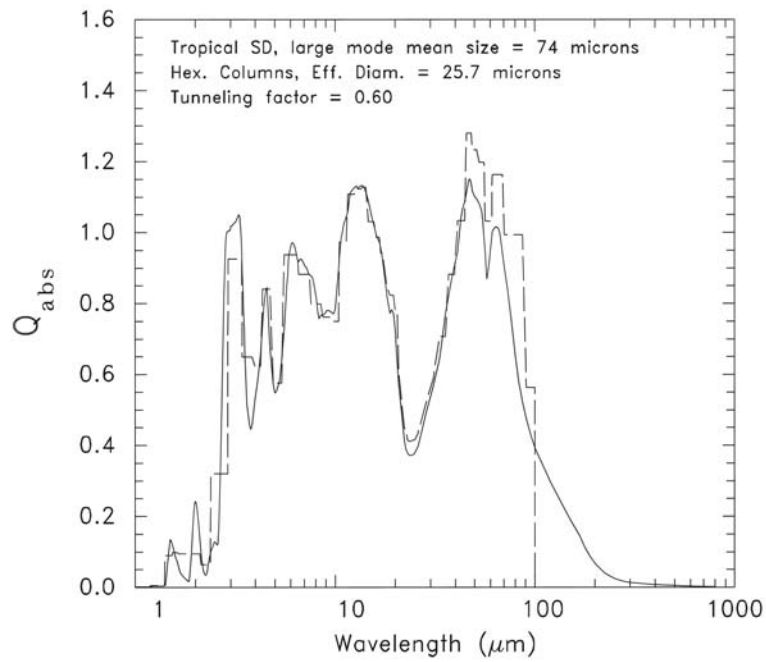


Figure 5. Comparison between the Fu schemes (dashed) and modified ADA for the conditions indicated regarding Q_{abs} .

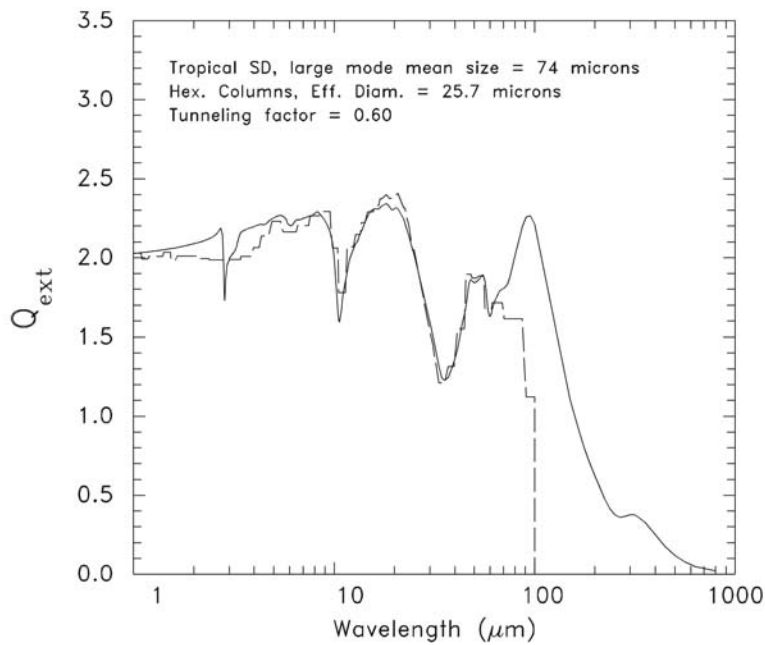


Figure 6. Comparison between the Fu schemes (dashed) and modified ADA (solid) for the conditions indicated, regarding Q_{ext} .

Mitchell (2002). It is not clear why this minimum is higher than the minimum at $\lambda = 5 \mu\text{m}$ regarding Fu et al., since the ice imaginary refractive index is lower at $\lambda = 4 \mu\text{m}$ than at $5 \mu\text{m}$. For extinction, percent differences are within 10% for all but the longest λ . Overall, the Fu scheme, which utilizes the FDTD method and the modified ADA scheme compare favorably.

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