# Approximations of polydispersed extinction

B. T. N. Evans and G. R. Fournier

A method to evaluate the polydispersed extinction efficiency rapidly is presented. The method can be used for any shape for which a monodisperse code or expression is known and any polydispersion for which a second moment inverse can be computed. Integration can be performed over any interval of the distribution function. Additionally, and if required, arbitrary accuracy can be obtained. This approach is applied to spheres and randomly oriented spheroids with $n$th-order log-normal and modified gamma particle distributions.

*Key words:* Extinction, scattering, aerosols, polydispersions. 

## 1. Introduction

The immediate objective of this study is to reduce significantly the computational burden of calculating the extinction from polydispersed particles—spherical or nonspherical.

Integrals over particle distributions are time-consuming to estimate by standard numerical techniques since the extinction efficiency must be calculated for each particle size before the integration over a particle size distribution can be performed. This can be unacceptable if large particle sizes or large optical sizes are involved. In addition, if nonspherical particles are considered, orientation distributions must be considered, adding another dimension to the problem. To accelerate the process we have derived an approximation that transforms the original integral into another integral that can be readily computed. Here, the particle distribution is absorbed into the integration variable and thus the numerical integration is optimally weighted.

Recent papers by Xing and Greenberg[1–3] give an efficient method for calculating the mean extinction that is based on the analyticity of the complex extinction efficiency. The method requires approximating the particle distribution by a function with simple poles. This provides excellent performance if the size distribution does not change frequently. Additionally, there would be significant complications if a finite interval were required.

Our method, although not without its own difficulties, overcomes the complications of the Xing and Greenberg approach when the particle size distribution is an $n$th-order log-normal or a modified gamma distribution. Since these distributions are rather general this is not normally a significant restriction. The most serious difficulty is to calculate the second moment inverse of the two distribution functions.

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Received 13 June 1995.
0003-6935/96/183281-05$10.00/0


## 2. Method

The definition of polydispersed extinction efficiency $\overline{Q}_{\text{ext}}$ is

$$\overline{Q}_{\text{ext}}(y) = \frac{\int_0^y x^2 Q_{\text{ext}}(x)\text{pdf}(x)\text{d}x}{\int_0^y x^2\, \text{pdf}(x)\text{d}x}, \tag{1}$$

where $y$ is the largest particle size parameter considered. In Eq. (1) $Q_{\text{ext}}(x)$ is the monodispersed extinction efficiency, pdf($x$) is the particle distribution function, and $x$ is the particle size parameter. As usual, $x = 2\pi r/\lambda$, where $r$ is the characteristic dimension of the particle and $\lambda$ is the wavelength of the source. The dimension $r$ for spheres is the radius and for spheroids the semiminor axis. For the log-normal and modified gamma distributions the integral in the denominator of Eq. (1) is algebraic. The integral in the numerator remains to be approximated.

The direct numerical integration of Eq. (1) has at least two problems associated with it. One is that $Q_{\text{ext}}$ can have a lot of high-frequency structure and the other is that pdf($x$) can have a long tail. Both situations cause computational difficulties since many integration points are required in any standard technique. By using an approximation[4] the first problem can be eliminated. To alleviate the long tail of the size distribution one must have a coordinate transform. We define the cumulative distribution function of the second moment of pdf($x$) as

$$\epsilon(z) \equiv \frac{\int_0^z x^2 \,\mathrm{pdf}(x)\mathrm{d}x}{\int_0^\infty x^2 \,\mathrm{pdf}(x)\mathrm{d}x}, \tag{2}$$

and its inverse function as

$$z(\epsilon) = \epsilon^{-1}(\epsilon). \tag{3}$$

Hence, $\epsilon$ is the fraction of the cumulative distribution from 0 to $z(\epsilon)$. From Eq. (2) it follows that

$$\mathrm{d}\epsilon(z) = \frac{z^2 \,\mathrm{pdf}(z)\mathrm{d}z}{\int_0^\infty x^2 \,\mathrm{pdf}(x)\mathrm{d}x}. \tag{4}$$

Therefore, we can write

$$\overline{Q}_{\mathrm{ext}}(y) = \frac{1}{\epsilon(y)} \int_0^{\epsilon(y)} Q_{\mathrm{ext}}(\epsilon)\mathrm{d}\epsilon. \tag{5}$$

This transformed integral has finite limits and uniformly weighs $Q_{\mathrm{ext}}$. Note that $\epsilon(\infty) = 1$. This form of integral is ideally suited for numerical evaluation, e.g., Gaussian quadrature.

Since we have $Q_{\mathrm{ext}}(x)$ and require $Q_{\mathrm{ext}}(\epsilon)$ we need the inverse function of $\epsilon$, $\epsilon^{-1}(z)$. If we consider the log-normal and modified gamma distributions, this requires inverses of their second moments. Since the indefinite integral of any log-normal distribution is known[5] and involves only the error function, its inversion is straightforward. (The inverse of the error function can be found in Section 26.2.22 of Ref. 6.) The inversion of the second moment of the modified gamma distribution is less straightforward.

We now define explicitly the log-normal and modified gamma distributions. The log-normal distribution is defined as

$$\mathrm{pdf}(x) = \left(\frac{x_j}{x}\right)^j \frac{\exp\{-(\ln[x/x_j]/\sigma)^2/2\}}{\sigma x_j \sqrt{2\pi}\,\exp[(j-1)^2\sigma^2/2]}, \tag{6}$$

where $x_j$ and $\sigma$ are the parameters that define the $j$th order log-normal distribution. The modified gamma function is defined as

$$\mathrm{pdf}(x) = \frac{x^{\sigma-1}\exp(-\beta x^\gamma)}{\gamma \beta^{\sigma/\gamma}\Gamma(\sigma/\gamma)}. \tag{7}$$

The parameters $\sigma$, $\beta$, and $\gamma$ are used to adjust the shape of the distribution. Increasing $\sigma$ increases the width and the peak position of the distribution. An increase of either $\beta$ or $\gamma$ decreases the width and peak position.

For the log-normal distribution $z(\epsilon)$ can be approxi-

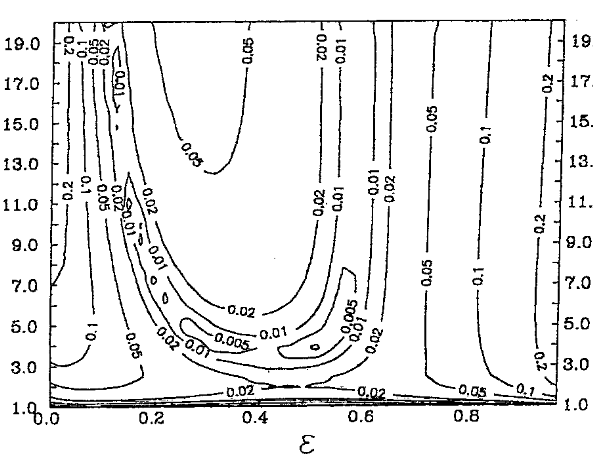


Fig. 1. Relative error of Eqs. (9), the first approximation to the inverse of the incomplete gamma function.

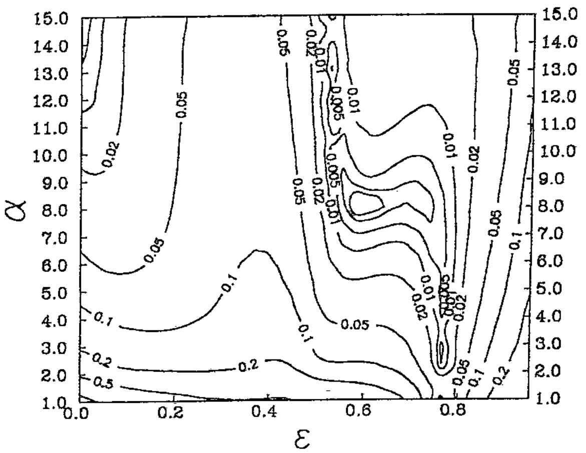


Fig. 2. Relative error of Eqs. (10), the second approximation to the inverse of the incomplete gamma function.

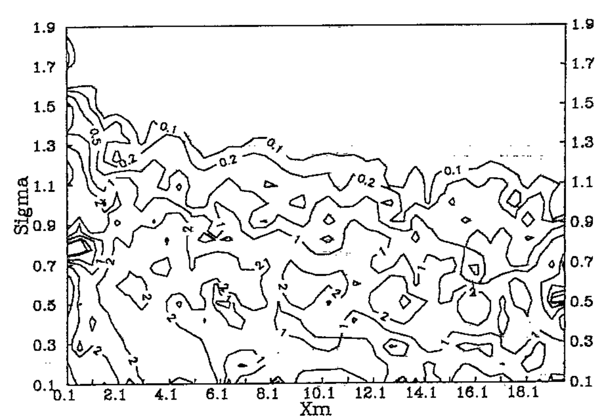


Fig. 3. Percent error of numerical approximation for the zero-order log-normal distribution.

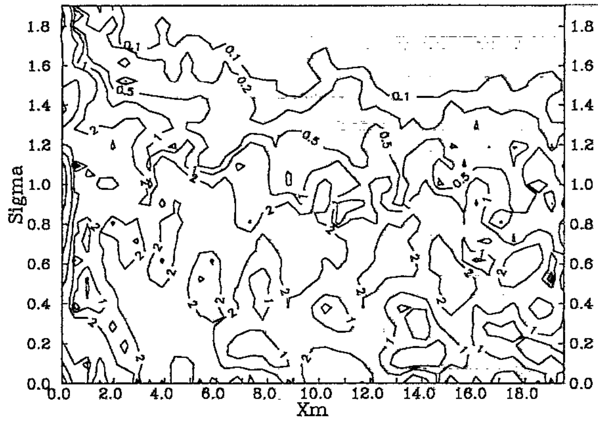


Fig. 4. Percent error of numerical approximation for the first-order log-normal distribution.

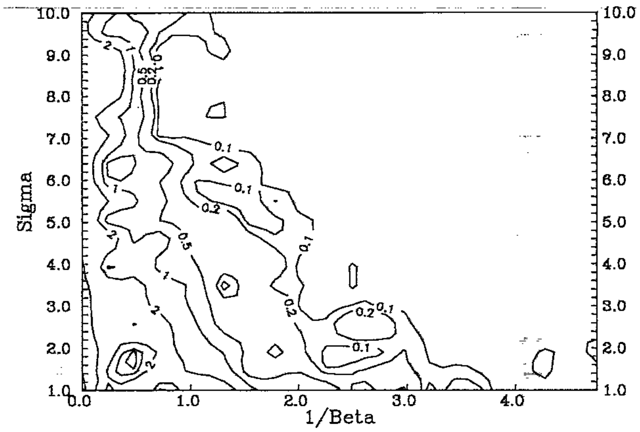


Fig. 6. Percent error of numerical approximation for the modified gamma distribution, $\gamma = 0.5$.

mated by

$$
\begin{aligned}
z(\epsilon) &= x_j \exp[(3 - j)\sigma^2 + p\sqrt{2}\sigma],\\
p &= \frac{1}{\sqrt{2}}\left(t - \frac{2.30753 + 0.27061t}{1 + 0.99229t + 0.04481t^2}\right),\\
t &= \sqrt{-2 \ln \epsilon}.
\end{aligned} \tag{8}
$$

For the modified gamma function, finding $z(\epsilon)$ requires the inverse of the incomplete gamma function, which has no efficient accurate numerical recipe.[7] We have hence produced two efficient schemes for computing this inverse function. They both start with a first-order approximation and then proceed by Newton's method of successive approximations. One starting approximation is simple but has inaccuracies as $\epsilon$ approaches one of its limits (either 0 or 1). The other is slightly more complicated, but for $\alpha > 4$ is superior to the first approximation. The first approximation, an *ansàtz* solution, is

$$
\begin{aligned}
z(\epsilon) &= \left[\frac{1}{\beta} \exp\{(\alpha - 1)\epsilon/[1 + (\alpha - 1)\epsilon]\}\left(\alpha\Gamma[\alpha]\ln\frac{1}{1-\epsilon}\right)^{1/\alpha}\right]^{1/\gamma},\\
\alpha &= \frac{\sigma + 2}{\gamma}.
\end{aligned} \tag{9}
$$

The second solution is derived by the uniform asymptotic expansion of the incomplete gamma function[7]:

$$
\begin{aligned}
z(\epsilon) &= \left(\frac{\alpha}{\beta c} Y\right)^{1/\gamma}, \quad \epsilon < 1/2,\\
&= \left[\frac{\alpha}{\beta c}(2c - Y)\right]^{1/\gamma}, \quad \epsilon > 1/2,\\
Y &= \left\{\frac{1 - \exp(-4/e)}{\exp(-5) - \exp(-4/e) + [1 - \exp(-5)]\exp(-4/c)}\right\}^{1/5},\\
c &= \exp(\eta^2 + 1),\\
\eta &= -\sqrt{2/\alpha}\,\mathrm{erfc}^{-1}(2\epsilon).
\end{aligned} \tag{10}
$$

Figures 1 and 2 show the errors of these two starting approximations. It can be seen from these figures that there are situations in which the error is large and hence the number of iterations in Newton's method is unacceptable. This situation, however, never occurs for both approximations under the same conditions. Hence, one or the other can always be used.

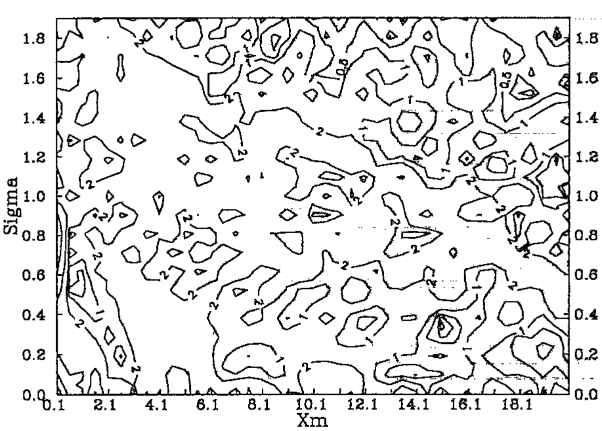


Fig. 5. Percent error of numerical approximation for the second-order log-normal distribution.

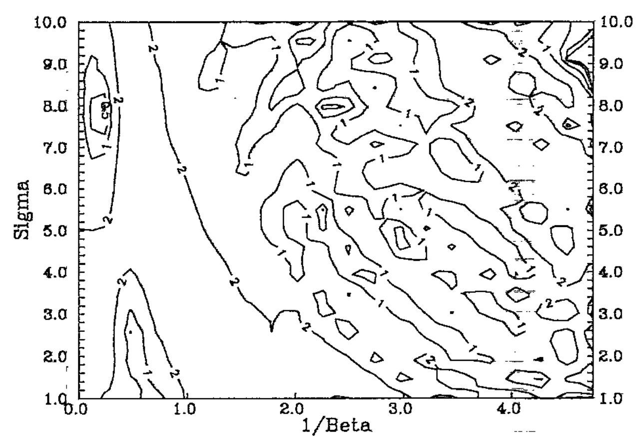


Fig. 7. Percent error of numerical approximation for the modified gamma distribution, $\gamma = 1$.

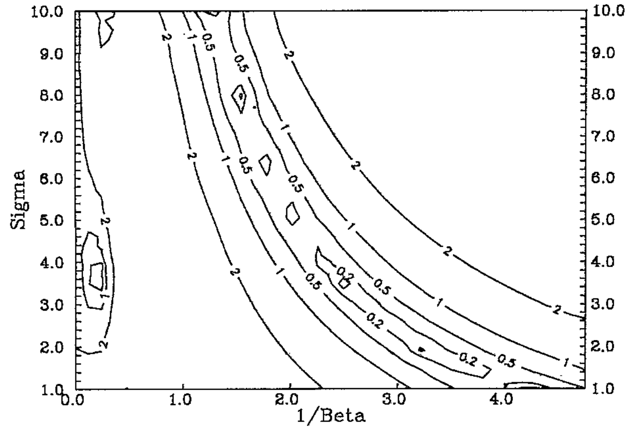


Fig. 8. Percent error of numerical approximation for the modified gamma distribution, $\gamma = 2$.

## 3. Results

We compare the approximation, using a seven-point Gaussian quadrature, with the exact calculation of $\overline{Q}_{ext}$ for spheres. The exact calculation being a 2000-point Gaussian quadrature of the size distribution over $Q_{ext}$ provided by a Mie routine. For convenience all the cases shown have integration limits from $\epsilon = 0.01$ to 0.99. In addition, this is close to the most time-consuming problem, which is $\epsilon = 0$ to 1. The refractive index is held constant at $m = 1.5\text{–}0i$.

Figures 3–5 are error diagrams for the three most common types of log-normal distribution. There are two general features to note. One is that as $\sigma \rightarrow 0$ the distribution tends to a Dirac delta function centered at $x_m$. Therefore, the bottom axis represents the error in a monodisperse aerosol and hence $Q_{ext}$. The other notable feature is that the error peaks along the $\sigma$ axis at a small value of $x_m$. These larger errors are a result of the error in $Q_{ext}$ in the transition region between the Rayleigh and anomalous diffraction limits. Because of the averaging process the peak error decreases with decreasing order of the distribution, specifically 5–12% for orders 0–2. The general error is seen to be much less than the peak error, typically 0.5–2%.

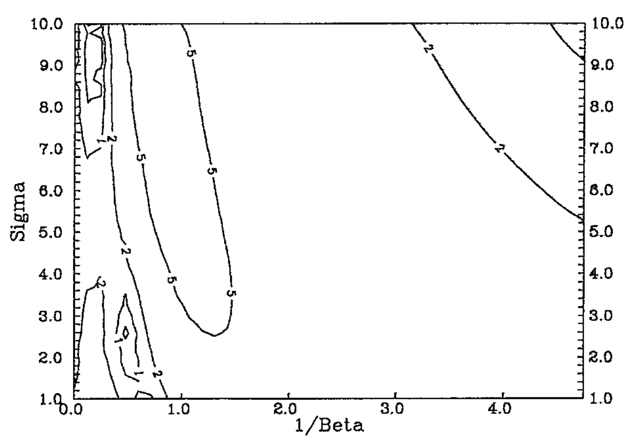


Fig. 9. Percent error of numerical approximation for the modified gamma distribution, $\gamma = 3$.

Figures 6–9 are similar error diagrams for the four most common types of modified gamma distribution that include the Deirmendjian distribution. As the location of the peak of the distribution varies as $1/\beta$ these diagrams are plots of $\sigma$ versus $1/\beta$. There is only one general feature to note, which is that the error peaks where the transition region is the major contributor to the total integral. This occurs when the peak of the second moment of the distribution is near 1. The peak error varies from 12% to 5% for $\gamma = 0.5\text{–}3$, the general error is typically 0.5–2%.

## 4. Discussion and Conclusions

The method can be readily extended to any particle type. The most important condition being that $Q_{ext}$ be computable for all the required $z$ values. A second condition, required to maintain reasonable accuracy and still be efficient, is that $Q_{ext}$ not vary rapidly with particle size (e.g., no large narrow resonances). Certain approximations, such as those based on anomalous diffraction, ensure that these two conditions are always satisfied.[4,8–10]

The approach allows more integration points to be added easily, thus the trade-off between speed and accuracy is simple. On an Intel i860 40-MHz (Microway NDP FORTRAN 860) as many as 400 values of $\overline{Q}_{ext}$ per second can be obtained. The 2000-point Gaussian on the exact Mie code with the same processor and compiler takes approximately 7000 s for the same 400 values. Using an algebraic approximation[4] for $Q_{ext}$ for randomly oriented spheroids, approximately 40 values of $\overline{Q}_{ext}$ per second can be obtained for any spheroid. From our previous experience with **T**-matrix codes for computing the exact extinction from randomly oriented spheroids, we estimate that the same 40 values would require in excess of 1000 h of computation time on the same processor.

It has been shown, by extensive computations, that typical errors are less than 2% when compared with exact calculations. Maximum errors are less than 12%. In applications for which accuracy is not of paramount importance, such as real field conditions, this error level is more than adequate.

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