Effects of smoothing and measurement-wavelength range on the accuracy of analytic eigenfunction inversions

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A smoothing technique is applied to improve the accuracy of inversions of Mie-extinction measurements with analytic eigenfunction theory. It is shown that a moderate amount of smoothing allows the inclusion of further terms, and thus extra information, in the expansion. The effects of measurement-wavelength range on the accuracy of inversions are also investigated, and it is shown that when large particles are present, measurements in the infrared region are necessary for accurate inversions.
Key words: Aerosols, inversion, remote sensing.

1. Introduction

The extraction of aerosol size distribution from multispectral extinction measurements is an inverse problem. Like many other inverse problems in remote sensing, it can be formulated in terms of a Fredholm integral equation of the first kind. This takes the form

$$\tau(\lambda) = \int_0^\infty \pi r^2 Q(r, \lambda, m) n(r) \mathrm{d}r, \quad (1)$$

where $\tau(\lambda)$ is the aerosol optical thickness (or extinction) at wavelength λ, Q is the Mie-extinction efficiency factor, m is the complex refractive index, and $n(r)$ is the aerosol size distribution.

The inversion of Eq. (1) is an ill-posed problem and is notoriously difficult. Ill posedness invariably leads to a loss of information and to highly unstable solutions. Also of importance is the fact that when solutions are obtained, they may be incomplete because the measurement kernels may be blind to a significant part of the function space of the unknown.

Some years ago McWhirter and Pike[1] developed an approach to inversion based on the Mellin transform of the kernel. Viera and Box[2] successfully used this approach with the anomalous diffraction approximation to Mie theory, assuming an infinite measurement range. This was later extended to the exact Mie-theory kernel and a finite measurement range.[3] In this paper we have used several synthetic data sets generated with a log-normal distribution to examine a number of aspects of the inversions.

A brief outline of analytic eigenfunction theory is given in Section 2. In expansion-type inversions such as this it is necessary to truncate the expansion at some point because the inclusion of further terms leads to oscillatory behavior. Section 3 outlines a smoothing method that we have used to reduce oscillatory behavior and thus allow the inclusion of more terms in the expansion. The results are given in Section 4 and show that a moderate amount of smoothing leads to improved retrievals, especially when a limited measurement-wavelength range is used.

The finite measurement-wavelength range used in our previous paper[3] was 0.368–2.250 µm, which is greater than the wavelength range available in many instruments. In Section 5 we present the results of an investigation into the effects of measurement-wavelength range on the quality of the retrievals. The ranges considered varied from 0.368–1.030 µm to 0.368–2.250 µm, and we found that for larger particles there is some loss of information with a limited measurement range.

When simulated data are used, it is easy to check the quality of retrievals by comparing the retrieved size distributions with the distribution used to generate the input data. With real data the only means of judging the validity of the retrieved size distribution is to use it to calculate the aerosol optical thickness

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and compare it with the input data. The aerosol optical thickness is defined by Eq. (1), but in practice integration will always be over a finite radius range. Section 6 gives the results of an investigation into the effects on calculated extinction of variations in the upper and lower integration limits. Generally, it was found that the integrations should be performed over the range 0.1–1.0 μm, at the very least, and varying the upper limit of the integration provided a way of establishing some degree of confidence in the retrievals.

2. Analytic Eigenfunction Theory

Details of analytic eigenfunction theory have been given elsewhere,[1–3] so only a brief outline is given here.

The generic Fredholm integral equation may be written as

$$g(x) = \int_0^\infty K(x, y) f(y) \mathrm{d}y, \qquad (2)$$

where $g(x)$ is the data function, $K(x, y)$ is the kernel, and $f(y)$ is the function to be retrieved. Analytic eigenfunction theory applies only to product kernels, that is, kernels of the form

$$K(x, y) = K(xy).$$

The Mie-theory extinction kernel is a product kernel if we write it as

$$Q(r, \lambda, m) = Q(kr, m),$$

where $k = 2\pi/\lambda$ and m is assumed to be constant.

The eigenfunctions and eigenvalues of such a product kernel are defined by

$$\int_0^\infty K(xy)\phi_\omega(x)\mathrm{d}x = \lambda(\omega)\phi_\omega(y). \qquad (3)$$

McWhirter and Pike[1] were able to construct $\lambda(\omega)$ and $\phi_\omega(y)$ by taking the Mellin transform of Eq. (3). They found that

$$\lambda(\omega) = |\tilde{K}(1/2 + i\omega)|,$$
$$\phi_\omega(y) = y^{(-1/2)-i\omega}\chi(\omega), \qquad (4)$$

where

$$\chi(\omega) = [\tilde{K}(1/2 + i\omega)/\pi\lambda(\omega)]^{1/2}$$

and $\tilde{K}(1/2 + i\omega) = \int_0^\infty t^{-(1/2)+i\omega}K(t)\mathrm{d}t$ is the Mellin transform of the kernel K.

The retrieval of $f(y)$ involves effectively expanding both it and $g(x)$ in terms of the eigenfunctions ϕ. $f(y)$ takes the form

$$f(y) = y^{-1/2}\,\mathrm{Re}\int_0^\infty G(\omega)y^{-i\omega}\chi(\omega)/\lambda(\omega)\mathrm{d}\omega, \qquad (5)$$

where

$$G(\omega) = \chi(\omega)\int_0^\infty g(x)x^{(-1/2)-i\omega}\mathrm{d}x.$$

Convergence requirements on the Mellin transform require selecting as the kernel

$$K(t) = \pi Q(t)/t,$$

with $t = xy = kr$. Therefore

$$f(y) \Rightarrow r^3 n(r),$$

and we identify y with r, and

$$g(x) \Rightarrow k^{-1}\tau(k),$$

and we identify x with k. Thus Eq. (2) becomes

$$k^{-1}\tau(k) = \int_0^\infty [\pi Q(kr)/kr][r^3 n(r)]\mathrm{d}r. \qquad (6)$$

The Mellin transform is obtained by numerical integration for values of ω from 0 to some maximum value, ω_m. The value of ω_m will depend on the level of error in the measurements and the nature of the underlying distribution.[2,4] In this paper a value of $\omega_m = 10$ has been chosen, as it was found that there were few changes in the retrieved distributions for values of $\omega_m > 7$.

A complex refractive index of $r = 1.5 - 0.01\, i$ has been assumed. This is a reasonable approximation for most aerosols.[5]

3. Smoothing

Any real measurements of multispectral optical thickness contain errors, even if they are only small. As can be seen from Eq. (5), the terms in the expansion are divided by the eigenvalues, which become smaller as ω increases, thus leading to increased error magnification. This can lead to instability in the solution of an expansion-type inversion as ω increases, and thus it is necessary to truncate the integration at some upper limit, ω_m. Truncation can lead to loss of information that may or may not be crucial.

In our earlier paper[3] the expansion was truncated at $\omega_m = 5.0$, but in this paper we look at the possibility of including the higher-order eigenfunctions in the solution by including a smoothing parameter S with values ranging between 0.0 and 0.10. Thus Eq. (5) becomes

$$f(y) = y^{-1/2}\,\mathrm{Re}\int_0^{\omega_m} G(\omega)y^{-i\omega}\chi(\omega)/\lambda'(\omega)\mathrm{d}\omega,$$

where

$$\frac{1}{\lambda'(\omega)} = \frac{\lambda(\omega)}{\lambda^2(\omega) + S\lambda(0)},$$

$\lambda(0)$ is the largest eigenvalue, and ω_m is the highest-order eigenfunction included. This method allows the value of ω_m to be increased and reduces the risk of severe oscillations as a result of errors in $g(x)$.

4. Effects of Smoothing

To investigate the effects of different levels of smoothing on the accuracy of inversions, a set of simulated data was generated by the use of Eq. (1) for measurement wavelengths 0.368, 0.500, 0.675, 0.862, 1.030, 1.250, 1.725, and 2.250 μm. These wavelengths are typical of those used in multispectral radiometers[6,7] and fall in atmospheric windows. A log-normal size distribution was assumed, and two mode-radius cases were considered, $r_m = 0.25$ μm and $r_m = 0.50$ μm, both with a spread parameter of 0.50. Data for two measurement-wavelength ranges, 0.368–1.030 μm and 0.368–2.250 μm, were inverted. The expansion for the retrieved function, $f(y)$, was truncated at $\omega_m = 10.0$. Three different values of the smoothing parameter S were tried: 0.0 or the unsmoothed case, 0.01 and 0.10.

Two methods of comparing the retrieved distribution with the true distribution were used. First, the retrieved volume-weighted size distribution, $f(y)$, was plotted and compared with the true distribution. Second, the values of $g(x)$ and $\tau(k)$ were calculated from the retrieved distribution and compared with the input values.

The graphical comparison of $f(y)$ with the true distribution showed that the broad features were the same regardless of the smoothing parameter used and agreed well with the true distribution. Major discrepancies tend to occur around the peak. The retrievals for the 0.368–2.250-μm range are given in Figs. 1 and 2.

In the case of $r_m = 0.25$ μm (Fig. 1) there was a tendency for the retrieved peak to shift to about 0.28 μm, regardless of smoothing parameter, so that agreement between the true distribution and the retrieved distribution was not too good for 0.15 μm $< r <$ 0.35 μm. For $S = 0.10$ the peak maximum was significantly underestimated, suggesting that much of the useful information in the later eigenfunctions has been lost. The picture is similar for $r_m = 0.50$ (Fig. 2), although the major discrepancies between the true distribution and the retrieved distribution are confined to the immediate peak region. It was found that $S = 0.0$ led to an overestimation of the peak and $S = 0.10$ led to an underestimation.

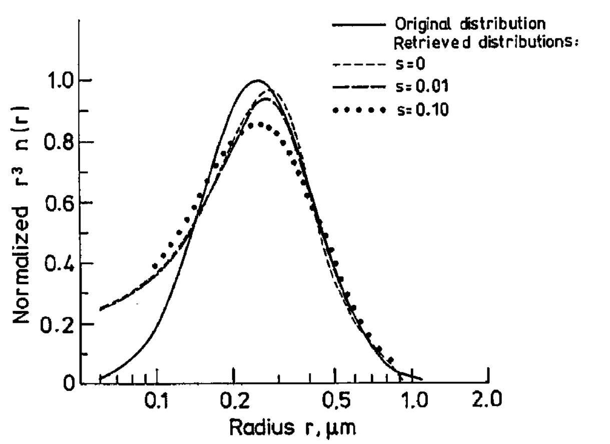

Fig. 1. Effect of the smoothing parameter on the accuracy of the retrieval for a log-normal distribution with mode radius $r_m = 0.25$ μm.

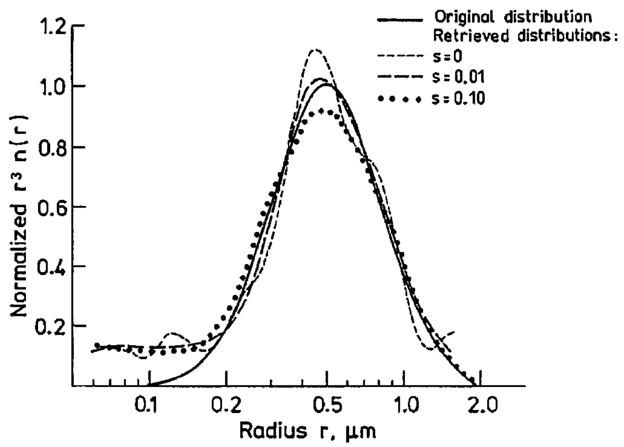

Fig. 2. Effect of the smoothing parameter on the accuracy of the retrieval for a log-normal distribution with mode radius $r_m = 0.50$ μm.

One of the advantages of using a smoothing parameter is that it removes the oscillatory behavior that appears when the value of ω_m is extended. There is little evidence of oscillatory behavior for $r_m = 0.25$, but Fig. 2 shows some oscillatory behavior in the $S = 0.0$ curve for $r_m = 0.50$. This behavior is not present in the $S = 0.01$ or $S = 0.10$ retrievals. The benefits of using a smoothing parameter become more apparent when a restricted measurement-wavelength range is used, both the $r_m = 0.25$ and $r_m = 0.50$ distributions exhibited oscillatory behavior in the unsmoothed case for the 0.368–1.030-μm range.

A second way of comparing the effects of the different smoothing parameters is to compare the input τ with the value of τ calculated with the retrieved volume-weighted size distribution. This is the only means of judging the accuracy of the retrieval that would be available in the case of real measurements.

Twenty sets of simulated data with 10% random error were generated for each size distribution and inverted. This allows us to examine the effects of random errors on the accuracy of the inversions as well as smoothing-related effects. The level of error used is higher than would be expected with a good radiometer, but undetected biases could result in errors as high as this. A high level of error also enables us to check the stability of the inversion. The results are summarized in Table 1 for the measurement-wavelength range 0.368–2.250 μm.

The original data, with no errors added, have been included in Table 1 along with the retrieved τ for these data for comparison. Examination of the results presented in the table shows that the differences

Table 1. Effect of Smoothing Parameter on Retrieved τ

λ (μm)	Input τ	10% Error, τ	Smoothing 0.00		Smoothing 0.01		Smoothing 0.10	
			No error	10% error	No error	10% error	No error	10% error
r_m = 0.25								
0.368	11.93	11.82 ± 0.69	11.53	11.72 ± 0.60	11.49	11.51 ± 0.50	11.25	11.21 ± 0.39
0.500	11.01	11.07 ± 0.50	10.75	11.05 ± 0.45	10.66	10.76 ± 0.36	10.27	10.25 ± 0.30
0.675	8.79	8.79 ± 0.63	8.65	8.93 ± 0.54	8.60	8.66 ± 0.43	8.29	8.26 ± 0.30
0.862	6.58	6.47 ± 0.35	6.47	6.71 ± 0.39	6.44	6.45 ± 0.31	6.29	6.23 ± 0.22
1.030	4.99	4.89 ± 0.27	4.94	5.21 ± 0.34	4.92	4.94 ± 0.23	4.88	4.82 ± 0.16
1.250	3.47	3.43 ± 0.21	3.43	3.78 ± 0.35	3.42	3.48 ± 0.21	3.47	3.43 ± 0.12
1.725	1.68	1.67 ± 0.11	1.64	2.02 ± 0.34	1.63	1.75 ± 0.18	1.73	1.72 ± 0.09
2.250	0.88	0.86 ± 0.03	0.79	1.09 ± 0.26	0.78	0.89 ± 0.13	0.85	0.86 ± 0.07
r_m = 0.50								
0.368	10.33	10.47 ± 0.63	10.28	10.48 ± 0.60	10.42	10.50 ± 0.57	10.55	10.62 ± 0.52
0.500	11.29	11.19 ± 0.66	11.24	11.38 ± 0.70	11.30	11.34 ± 0.59	11.27	11.33 ± 0.46
0.675	11.92	12.17 ± 0.68	11.78	12.09 ± 0.71	11.83	11.95 ± 0.55	11.53	11.62 ± 0.38
0.862	11.64	11.67 ± 0.57	11.80	11.88 ± 0.39	11.60	11.75 ± 0.36	11.12	11.25 ± 0.30
1.030	10.83	10.96 ± 0.60	10.71	11.00 ± 0.33	10.70	10.87 ± 0.32	10.21	10.36 ± 0.27
1.250	9.41	9.69 ± 0.44	9.32	9.70 ± 0.44	9.34	9.53 ± 0.38	8.94	9.09 ± 0.30
1.725	6.46	6.54 ± 0.44	6.22	6.67 ± 0.56	6.33	6.49 ± 0.43	6.13	6.25 ± 0.23
2.250	4.30	4.38 ± 0.22	3.75	4.10 ± 0.50	3.88	3.98 ± 0.36	3.79	3.87 ± 0.16

between the retrievals with no error and those with 10% error are within one standard deviation, and thus we can conclude that the presence of error in the input data has no significant effect on the accuracy of the retrieval.

When the different levels of smoothing are compared, we note that the standard deviation for the calculated τ decreases as S increases. The results presented are for $\omega_m = 10.0$. Examination of the results for other values of ω_m shows that with $S = 0.10$ there was little change in the value of τ after $\omega = 5.0$. This suggests that a smoothing parameter of 0.10 may be a little high, as it is effectively masking out much of the information contained in the later eigenfunctions.

When errors in the input data and the retrieved τ are taken into account, we find that satisfactory retrievals are obtained for all levels of smoothing. With a smoothing of 0.10 the calculated τ were generally a little low, which would be expected when the size-distribution peak is underestimated.

Although the differences between the retrievals with different smoothing parameters are probably not statistically significant, it does appear that some smoothing is useful. Overall the results for $S = 0.01$ appear to be the best, and this value has been used in the rest of the research reported here.

5. Effects of Wavelength Range on Retrieved Distribution

Measurements of aerosol optical thickness are not taken over an infinite range of wavelengths but are taken at a number of discrete points. The number of measurements available, the particular wavelengths used, and the total wavelength range vary with the instruments and the purpose of the investigation.

In this section the set of simulated data points, generated as outlined in Section 4, is used to examine the effects of wavelength range on the accuracy of inversions. Three measurement groupings were considered: 0.368–1.030 μm, 0.368–1.725-μm, and 0.368–2.250 μm. The results presented are for $\omega_m = 10.0$ and a smoothing parameter S of 0.01.

It is known that the particle sizes that can be retrieved depend on the measurement-wavelength range. Earlier research by Viera and Box[4] showed that the extinction experiment is effectively blind to particles smaller than 0.1 μm and larger than 2.0 μm. In this study we compare the retrieved volume-weighted distribution with the true distribution and also the calculated value of τ (calculated with this distribution) with the input value. The results presented use integration over the radius range 0.1–1.4 μm for τ. [In cases in which $f(y)$ becomes negative before 1.4 μm, the integration is truncated at that point.]

Considering first the distribution with a mode radius of 0.25 μm, one can see that plots of the retrieved distribution versus radius showed very little difference between the retrieved volume-weighted distributions for the three wavelength ranges considered. All three retrievals show a shift in the peak to 0.28 μm and underestimate the peak value by 2–5%. The main difference in the distributions is the sharp drop-off at the large-particle end for the 0.368–1.030-μm range.

Table 2 gives the input and the calculated τ for the three wavelength ranges. In most cases the calculated values are quite good, with the retrieved distribution accounting for 95% or more of the observed extinction. The addition of extra measurements in the infrared region led to an improvement in the calculated τ for the smaller wavelengths.

When we consider the distribution with a mode radius of 0.50 μm, we show that the measurement range has a marked effect on the accuracy of the retrieved distribution. The retrieved distributions and the true distribution are plotted in Fig. 3. It can be seen from the figure that the restricted wavelength range, 0.368–1.030 µm, results in a very poor retrieval. The peak is grossly overestimated, and the distribution drops off very rapidly at the large-particle end. These deficiencies are largely overcome with the addition of the infrared wavelengths. With the 0.368–1.725 µm measurement set there is still some overestimation of the peak and the distribution drops off more rapidly than the true distribution for $r > 1.2$ µm, but elsewhere the agreement is very good. The agreement between the retrieved distribution and the true distribution is very good over the whole range when the measurement at 2.25 µm is included.

Comparison of observed (input) and calculated optical thicknesses in Table 2 shows the same trends. The 0.368–1.030-µm distribution leads to an overestimate of τ; the addition of infrared measurements leads to an improvement in the calculated τ, which is most marked for the addition of the measurement at 2.25 µm, although the retrieved value for τ (2.25 µm) is significantly worse than the rest, as was the case for the $r_m = 0.25$ distribution.

The general conclusion to be drawn from this is that the analytic eigenfunction method is capable of giving good inversion results for small particles when the measurement range is restricted to wavelengths less than 1 µm. If the particles in the distribution are larger, then measurements in the infrared are necessary if good results are to be obtained.

6. Effects of Integration on Calculated τ

In order to get some idea of how well the retrieved size distribution accounts for the input data it is necessary to integrate the distribution over a suitable range of r to calculate τ. As has been mentioned above, the extinction experiment is effectively blind to particle sizes below 0.1 µm, and at the upper end of the range the fit becomes poor at different radii, depending on the measurement-wavelength range and the underlying distribution.

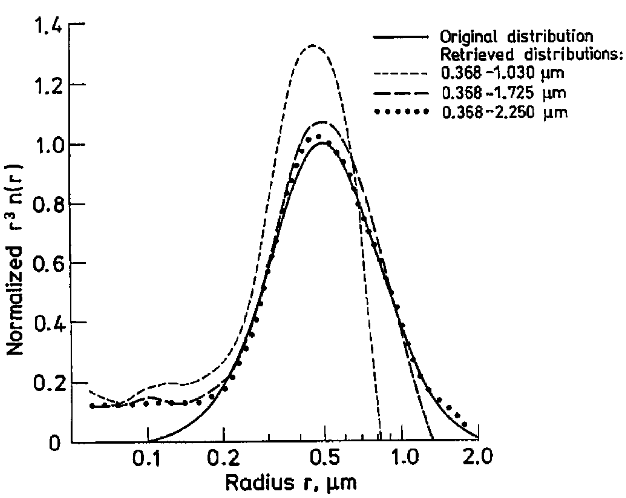

Fig. 3. Effect of the measurement-wavelength range on the accuracy of retrieval for a log-normal distribution with mode radius $r_m = 0.50$ µm.

Table 2. Effect of Measurement Range on Calculated τ

		Calculated τ		
λ (µm)	Input τ	1.030 µm	1.725 µm	2.25 µm
r_m = 0.25 µm				
0.368	11.93	11.80	11.53	11.49
0.500	11.01	11.01	10.70	10.66
0.675	8.79	8.96	8.65	8.60
0.862	6.58	6.68	6.49	6.44
1.030	4.99	5.05	4.97	4.92
1.250	3.47		3.46	3.42
1.725	1.68		1.65	1.63
2.250	0.88			0.78
r_m = 0.50 µm				
0.368	10.33	11.45	10.79	10.42
0.500	11.29	12.40	11.64	11.30
0.675	11.92	13.20	12.21	11.83
0.862	11.64	12.36	12.06	11.60
1.030	10.83	10.60	11.17	10.70
1.250	9.42		9.71	9.34
1.725	6.46		6.40	6.33
2.250	4.30			3.88

We looked at a number of different integration ranges in order to determine how critical this was to the calculated τ. It was assumed that the contribution to the integral outside this range was zero.

Two different lower limits were used, 0.1 and 0.16 µm, and in both the $r_m = 0.25$ µm and the $r_m = 0.50$ µm distribution, the 0.16-µm limit gave a poorer result. This would obviously be expected for $r_m = 0.25$ µm, as it results in the loss of a significant portion of the distribution. The effect was less pronounced for the $r_m = 0.50$ µm distribution but was still noticeable.

Four different upper limits were used: 0.80, 1.0, 1.2, and 1.4 µm. For both distributions there was an improvement in calculated τ when the limit was raised from 0.8 to 1.0 µm. This improvement continued as the upper limit was increased to 1.2 and then 1.4 µm for the $r_m = 0.50$ µm distribution. This would be expected when we look at the underlying distribution; there are still a significant number of particles in this region. (When the retrieved distribution becomes negative before the upper limit is reached, the integration is truncated.)

These results suggest that there is some value in using variable integration limits when calculating τ from the retrieved distribution. Such limits provide a means of determining the size range over which the most confidence can be placed in the inversion. The values of τ given in Tables 1 and 2 are for $\omega_m = 10.0$, although the integrations were done for $4.0 < \omega_m < 10.0$, and examination of the results shows that τ is generally stable for $\omega_m > 7.0$. Performing the integrations for a number of different values of ω_m provides us with another way of judging the quality of the inversions by indicating when the addition of further terms in the expansion makes little contribution to the final result.

7. Summary and Conclusions

Previous research has established the value of analytic eigenfunction theory for the inversion of aerosol optical-thickness data. In this paper it has been shown that the addition of a smoothing parameter in the expression for the retrieved distribution can lead to better results by allowing more terms to be included in the expansion. This smoothing parameter effectively dampens the effects of increased error magnification that occur with higher-order eigenfunctions while allowing some of the extra information contained in them to be included.

The smoothing parameter does not, and indeed should not, change the major features of the retrieved distribution. Our results show that only a moderate amount of smoothing is necessary for best results. Smoothing proved to be most effective in producing more accurate retrievals when a restricted measurement-wavelength set was being used to retrieve a size distribution with a significant number of larger particles.

The effect of measurement-wavelength range on the accuracy of size-distribution retrievals was clearly demonstrated in Section 5. Although a restricted wavelength range is adequate for small particle sizes, it is necessary to include measurements in the infrared part of the spectrum if larger particles are present. The presence of larger particles than can effectively be resolved by the use of the measurements that are available is evidenced by a sharp drop-off at the large-particle end, such as was the case in Fig. 3 for the 0.368–1.030-μm data set. The sharp drop-off results from the fact that analytic eigenfunction theory makes no assumptions about the underlying distribution.

With simulated data it is easy to compare the retrieved distribution with the true distribution when evaluating the accuracy of an inversion. In the case of real data this option is not available; instead the retrieved distribution may be used to calculate the aerosol optical thicknesses at the measurement wavelengths. The better the agreement between the observed and calculated values, the better the fit. When one is calculating the extinctions, it is necessary to integrate over a finite radius range. It is not always easy to select the best range, but our results show that a lower limit of 0.1 μm should be used, and there is some value in varying the upper limit to determine when no further improvement is obtained.

Another factor affecting the accuracy of the inversion is the value at which the expansion is truncated, ω_m. This truncation limit will also affect the calculated optical thicknesses, with significant improvements up to some value of ω_m, which may vary from one data set to another, and little improvement for larger values. By calculating the optical thicknesses for various values of ω_m, and for varying integration ranges, both of which are easily incorporated in the inversion process, we effectively obtain a set of solutions. Comparison of these solutions provides further means of judging the accuracy of the inversion.

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