

Apodization effects in the retrieval of volume mixing ratio profiles

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In remote sensing applications, spectra measured by Fourier-transform spectrometers are routinely apodized. A rigorous analysis approach would explicitly account for correlations induced in the covariance matrix by apodization, but these correlations are often ignored to simplify and speed up the processing. Using spectra measured by the Atmospheric Trace Molecule Spectroscopy missions, we investigated the effect of apodization on the retrieval of volume mixing ratio profiles for the case in which these correlations are ignored. Minor discrepancies occur between results for apodized and unapodized spectra, particularly when lines with a low signal-to-noise ratio are fitted. A set of microwindows is reported for O₃ in the range of 1550–3350 cm⁻¹. © 2002 Optical Society of America

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1. Introduction

The Atmospheric Chemistry Experiment (ACE)¹ is a satellite mission developed under the auspices of the Canadian Space Agency and is scheduled for launch in December 2002. The primary goal of the ACE mission is to investigate the chemical and dynamical processes that control the distribution of ozone in the stratosphere and upper troposphere, with a particular focus on the Arctic winter stratosphere. The primary instrument on board the satellite is a Fourier-transform spectrometer (FTS) operating between 2 and 13 μm with an unapodized resolution of 0.02 cm⁻¹. Also on board is a pair of filtered imagers (square complementary metal-oxide semiconductor detector arrays recording images of the Sun) operating at 1.02 and 0.525 μm and a UV-visible spectrometer operating between 0.285 and 1.03 μm with a resolution of 1–2 nm.

The measurement technique to be used is the well-known solar occultation spectroscopy method. As the satellite progresses in its orbit, it will see the Sun rise and set up to 16 times per calendar day. Over the course of a sunrise or sunset event (i.e., an occul-

tation), instruments on the satellite will measure transmission of sunlight for several different paths through the Earth's atmosphere. From these measurements, variations as a function of altitude will be inferred for pressure, temperature, aerosols, and the volume mixing ratios (VMRs) of approximately 30 molecules.

As with any FTS,² the issue of apodization and its effect on the data analysis must be considered for the ACE FTS. Because of the (necessarily) finite extent of FTS scans, the FTS output suffers what is referred to as truncation error: The output stops abruptly at the end of the recording, and the Fourier transform of the resulting clipped function exhibits ringing for sharp spectral features. The finite scan time can be represented by a windowing operation (in this case, a rectangular or boxcar function of time) on the data in the Fourier analysis. In Fourier spectrometry, apodization denotes use of alternate windowing functions to artificially reduce the effects of abruptly ending the FTS recording and thereby suppress the ringing of FTS signals.

Apodization has been shown to have consequences on the validity of Beer's law,^{3,4} belying the common tacit assumption that apodization is benign and therefore has no effect on the analysis results. Because the observed and calculated spectra are always processed in the same manner, apodization may indeed have little impact, but it is dangerous to just assume so for such a highly nonlinear process. Potential problems (or benefits) arising from apodization must receive due consideration when one is evaluating an analysis approach.

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2. Apodization

The original intent of apodization was to satisfy aesthetics, to suppress the ringing, and to provide a smooth output that looked more like the output of scanning spectrometers. As a side benefit, the apodization process reduced the computational requirements of analysis, essentially by decreasing the frequency range associated with sharp lines. The sidelobes of the FTS sinc line-shape function decrease in amplitude only as the reciprocal of the detuning from line center. Apodization concentrates the signal in a narrower frequency range, which is computationally less expensive to model. Currently, most spectral analysis is done on computers, which have no sense of aesthetics and care naught for how smooth the spectrum is; also major advances in computing power have decreased the need (in terms of minimizing computing time) for preprocessing the FTS spectra. Despite these facts, apodization has remained entrenched as standard practice in the field of Fourier-transform spectroscopy, particularly in the community of atmospheric remote sensing.

There are many different apodization approaches, too varied to describe in any detail here. One can even fine tune the windowing function to a specific application.^{5,6} In the field of FTS remote sensing, perhaps the most common form of apodization used is known as Norton–Beer apodization.⁷ Three common variations of Norton–Beer apodization—weak, medium, and strong, otherwise known as Norton–Beer apodization 1, 2, and 3, respectively—permit different degrees of severity for the attenuation of FTS sidelobes.

Apodized spectra suffer a linewidth broadening. To avoid the associated loss of spectral resolution, the ACE team has decided not to use apodization. Implications of this decision are investigated here.

3. Analysis

Heritage software originally from the Jet Propulsion Laboratory⁸ has been adapted and updated by members of the ACE Science Operations Center, located at the University of Waterloo. Software development has progressed with the Atmospheric Trace Molecule Spectroscopy (ATMOS) data set used as a baseline. The ACE software uses a global-fit type approach⁹ for the retrieval of VMR profiles of atmospheric constituents, as compared with the onion peeling approach¹⁰ used in the heritage software. The nonlinear least-squares routine in the software makes use of the Levenberg–Marquardt algorithm.¹¹ The analysis software uses the standard approach of fitting microwindows, small ($\sim 1 \text{ cm}^{-1}$ wide or smaller) portions of the spectrum that contain spectral features primarily from the molecule of interest; frequency and altitude ranges for the microwindows are chosen to minimize contributions from interfering species.

In a previous investigation by Amato *et al.*,¹² it was concluded that apodization had no effect on the retrieval of geophysical parameters. It is important to note that Amato *et al.* were careful to propagate for-

ward the effect of apodization on the covariance matrix of the observations. Apodization correlates points in the spectrum, and one must account for the effect on the covariance matrix to properly weight the least-squares fit. Unfortunately, for a high-resolution instrument such as the ACE FTS, analysis of a single occultation involves tens of thousands of data points, even with use of microwindows, and properly accounting for apodization-induced correlations is a cumbersome and time-consuming process. Operational processing for a mission with a relatively high data rate (such as the ACE mission, which will measure a new occultation approximately every 45 min) can ill afford such complications. This is yet another incentive (i.e., aside from the issue of spectral resolution) for the ACE mission to adopt the analysis of unapodized spectra.

Historically (and currently), in the field of atmospheric remote sensing, analysis software has avoided the complications of apodization-induced correlations by simply neglecting the effect (except perhaps to modify the error bars on the final results). This includes both ATMOS version 2 and ATMOS version 3¹³ processing. One aspect of the verification process for the ACE software will be to compare the results of ATMOS data to published ATMOS version 2 and ATMOS version 3 results, both of which routinely used Norton–Beer apodization during analysis. It is therefore instructive to consider what effects (if any) arise from the analysis of apodized spectra without having to explicitly account for the induced correlations. Thus all fittings in the current paper use the same diagonal covariance matrix for the data, i.e., treat each point in a spectrum as being independent and assign it a common uncertainty ($1/70$ in transmittance units), regardless of whether the spectrum is apodized or unapodized.

Rather than using synthetic spectra, we performed the processing on ATMOS experimental data. It was a simple test case that implicitly contained all the complicating factors one would expect for the ACE data set, with no need to make assumptions concerning the origin or distribution of errors and no need to model esoteric effects that could have some influence on the results (e.g., smearing of the interferogram because of a changing scene over the course of a single scan,¹⁴ resonant dispersion effects, corrections for detector nonlinearity).

A portion of the ATMOS data set was analyzed with the ACE software. VMR profiles were retrieved for seven different molecules (O_3 , CH_4 , N_2O , H_2O , NO_2 , CO_2 , and HCl) that have signals in the $1550\text{--}3350\text{-cm}^{-1}$ range, the filter 3 region for ATMOS. Occultations from more than one mission were analyzed to avoid systematic errors. Temperature and pressure profiles were taken from ATMOS version 2 results.¹⁵ In general, results with and without apodization were quite consistent, with only minor discrepancies (typically within 2σ error bars). Details of the discrepancies that were observed are described below.

For CH_4 and N_2O , discrepancies between results

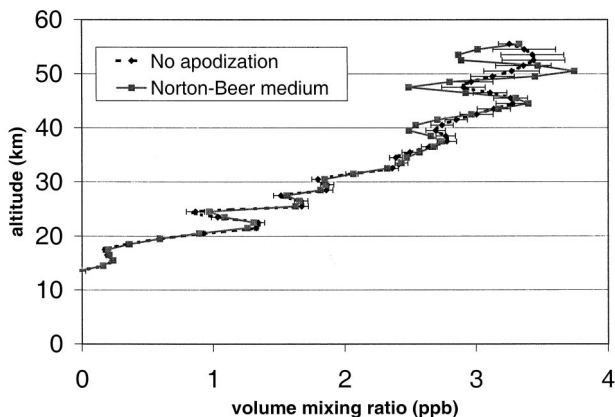


Fig. 1. HCl retrieval with and without apodization for ATMOS ATLAS-1, sunset 16. Error bars are shown for one data set only. Results from analysis of the apodized spectra often exhibit more of an oscillatory behavior. ppb, parts per billion.

with and without apodization were typically less than the 1σ error bars—except in a few isolated cases—and showed no systematic behavior in the deviations.

Results for H_2O , CO_2 , and HCl often showed discrepancies of the order of 2σ error bars (i.e., the 1σ error bars for the two results barely overlapped), and the discrepancies were systematic for these molecules. An example is given in Fig. 1, which shows two retrieved VMR profiles for HCl on a common plot. We performed the analysis using the ACE software on data from sunset 16 of the ATLAS-1 (Atmospheric Laboratory for Applications and Science) mission. To avoid clutter, error bars in Fig. 1 are shown for only one result; error bars for the other result are roughly equal in size. The error bars are the standard 1σ uncertainties from the square root of the diagonal elements in the parameter covariance matrix. These errors are possibly underestimated (because effects from parameter nonlinearities¹⁶ are not accounted for in this approach) but are sufficiently accurate for the current purposes.

For the two retrievals shown in Fig. 1, we obtained one profile from fitting unapodized spectra and the other from analyzing the same spectra processed by Norton–Beer medium apodization. Note in particular the discrepancies at higher altitudes. Results at the higher altitudes come from when the lines are fit with a low signal-to-noise ratio. Oscillations in the VMR profile at high altitudes arise from the fact that one is working at the limit of information content. Thus these oscillations are numerical artifacts and are not physically significant, and it is certainly acceptable for one to smooth the results by imposing regularization, as will be done by the Michelson interferometer for passive atmospheric sounding.¹⁷ However, note that the unphysical oscillatory behavior is significantly reduced when we fit the unapodized spectra. Similarly, oscillations in the results for CO_2 and H_2O are also reduced when we work with unapodized spectra. The greatest improvements in the smoothness of results occur at altitudes for which

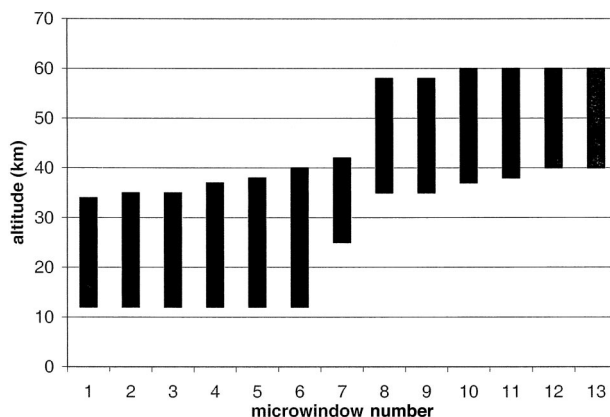


Fig. 2. Altitude ranges for the microwindows used in the ATMOS version 2 retrievals of ozone.

the fitted data consist primarily of weak lines (signal-to-noise ratio the order of 10:1 or worse).

There are no plans to implement regularization in the ACE software because it would merely represent an aesthetic improvement to the appearance of the profile and also would interfere in the determination of a true error estimate for the fitting parameters (i.e., that takes the effect of parameter nonlinearities into account, not just the square root of the diagonal elements of the variance–covariance matrix). Simply choosing to analyze unapodized spectra seems to damp out unphysical oscillations in the fitted VMR profiles to a significant degree, making use of regularization somewhat redundant.

The results for O_3 often showed discrepancies of the order of the 1σ error bars. Unfortunately these discrepancies were usually for altitudes near the peak of the VMR profile. For most molecules, it is impossible to find microwindows that span the entire altitude range of interest. Figure 2 shows a bar graph depicting the altitude ranges of microwindows in the ATMOS filter 3 ($1550\text{--}3350\text{-cm}^{-1}$) region used in the ATMOS version 2 analysis of ozone. The im-

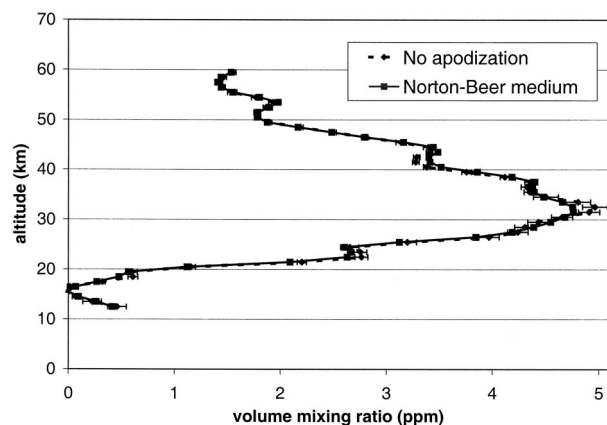


Fig. 3. O_3 retrieval with and without apodization, ATMOS ATLAS-3, sunrise 47. Error bars are shown for one data set only. Discrepancies exist in the vicinity of the peak. ppm, parts per million.

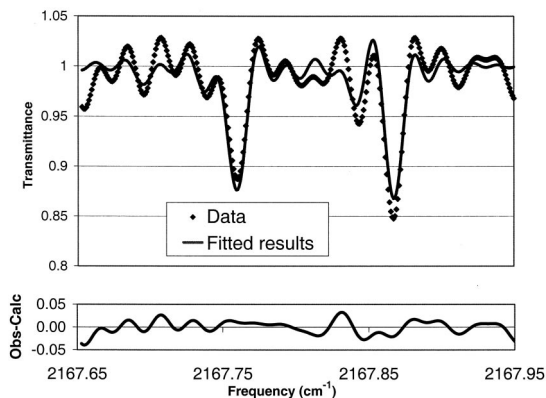


Fig. 4. ATMOS ATLAS-3, sunrise 47, tangent height 35.2 km, center frequency 2167.8 cm^{-1} , microwindow width 0.3 cm^{-1} , no apodization. Observed and calculated spectra are plotted in the upper graph, and residuals are plotted in the lower graph.

portant 30–38-km altitude region (the VMR peak of ozone) is at or near the upper limit for several of the microwindows. Thus the VMR of ozone determined for this region comes mostly (although not entirely) from the fitting of weak lines. This is far from the ideal situation.

Figure 3 shows two retrieved profiles for O_3 from sunrise 47 of the ATLAS-3 mission, one from the analysis of unapodized spectra and the other from analysis of spectra processed with Norton–Beer medium apodization. Again, to avoid clutter, error bars are shown for only one result. Note the discrepancies near the VMR peak. Figure 4 shows the fitted result without apodization for a particular ozone microwindow and for a tangent height near the VMR peak of ozone. Figure 5 shows the result for the same microwindow, but with Norton–Beer medium apodization. Note the significant broadening of the spectral features that results when apodization is applied.

The final molecule under consideration, NO_2 , fared

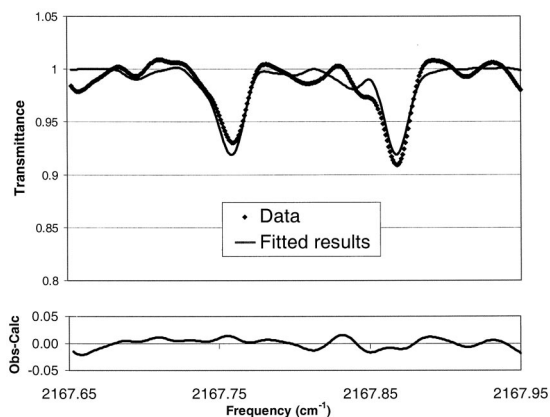


Fig. 5. ATMOS ATLAS-3, sunrise 47, tangent height 35.2 km, center frequency 2167.8 cm^{-1} , microwindow width 0.3 cm^{-1} , Norton–Beer medium apodization. Observed and calculated spectra are plotted in the upper graph, and residuals are plotted in the lower graph.

the worst of all. Discrepancies were often of the order of the 2σ error bars or larger and again were well correlated with the fitting of primarily weak lines (in this case, near and above the VMR peak for the molecule).

It should be noted that the discrepancies are not instabilities in the fitting. For a given apodization, the software converges to the same result regardless of initial guess, including poor initial guesses (e.g., a constant vertical profile).

4. New O_3 Microwindows

O_3 is without question the most important molecule in stratospheric studies. Thus it is worth considering whether the consistency for this molecule can be improved. Because the problem appears to be use of mostly weak lines for altitudes near the VMR peak, the obvious solution is to make a more judicious choice of microwindows that avoids (as much as possible) weak lines.

In addition to providing mostly weak lines for the most important altitudes, the microwindows used for ATMOS version 2 results also suffer significant interferences from other molecules. A new set of microwindows for ozone in the frequency range $1550\text{--}3350 \text{ cm}^{-1}$ is presented in Table 1. Note that these microwindows are optimized for the ATMOS instrument and may need to be adjusted (e.g., slightly different altitude ranges) when it comes time to analyze data from the ACE FTS.

Interferences in the new microwindows were carefully avoided, allowing no more than 1–2% absorption for interfering species (as compared with more than 20% for many of the old ATMOS version 2 microwindows). Each new microwindow contains a stretch of baseline, i.e., a portion with little to no absorption, not an easy criterion to meet with the dense ozone spectrum. Another criterion used in the microwindow selection process was temperature sensitivity: Lines with high lower-state energies were avoided. This minimizes the propagation of errors from temperature determination. Blended ozone lines were also avoided as much as possible. Great care was taken to have enough microwindows (approximately 15, where possible) at any given altitude to give good statistics in the fitting process. Lower limits on altitude ranges were chosen to avoid deformation of the line shape by saturation. Upper limits on the altitude ranges were chosen such that the ozone lines contained within had at least 20% absorption under relatively low-ozone conditions (which was the case for sunrise 47 of ATLAS-3, as is evident in Fig. 3 to those familiar with atmospheric ozone). For the ATLAS series of missions, this corresponds to a signal-to-noise ratio of approximately 15.

Problems with apodization effects are reduced when we use this new microwindow set. This can be seen in Fig. 6, which shows retrievals with and without apodization for sunrise 47 of ATLAS-3 by use of the new microwindow set. There are still differences, but the discrepancies are more subtle than those obtained with the old microwindow set. Note

Table 1. O₃ Microwindow Set for the 1550–3350-cm⁻¹ Region

Center Frequency (cm ⁻¹)	Width (cm ⁻¹)	Altitude Range (km)
1803.30	0.40	12–32
1811.80	0.60	25–38
1814.28	0.45	25–39
1815.78	0.30	25–39
1819.52	0.55	12–32
1833.89	0.45	12–35
1836.30	0.50	16–31
2010.70	0.30	12–25
2012.58	0.30	12–25
2085.81	0.30	36–52
2091.28	0.30	38–52
2092.71	0.40	38–54
2095.20	0.40	40–55
2095.97	0.45	44–55
2098.27	0.35	44–55
2115.32	0.30	43–52
2116.05	0.26	44–55
2120.02	0.40	43–55
2120.66	0.32	42–55
2121.67	0.35	48–55
2122.23	0.35	44–55
2123.40	0.30	44–55
2126.53	0.45	39–55
2127.18	0.30	36–52
2145.78	0.30	12–25
2150.15	0.30	17–33
2152.99	0.35	20–32
2778.99	0.43	15–36
2997.50	0.40	22–34
3019.71	0.30	33–43
3023.47	0.40	32–43
3026.47	0.45	25–43
3026.85	0.35	35–44
3028.04	0.40	35–44
3031.49	0.25	31–44
3032.52	0.50	33–44
3035.29	0.80	25–44
3041.00	0.40	25–43
3041.57	0.55	32–40
3057.38	0.30	34–43
3058.53	0.40	25–42
3092.17	0.30	17–30
3190.76	0.30	12–25

that the microwindows were conservatively chosen and could be extended above 55 km; for the ACE mission, however, results at altitudes higher than 55 km will be obtained when microwindows are fitted in the 10- μ m band of ozone.

In addition to the (relative) insensitivity to apodization effects, there are additional benefits to the new microwindow set. With the old microwindow set, there was a tendency for the retrieved VMR profile to dip into negative values below 15 km. The new set fixes this problem. The fit itself is also much better. For no apodization, the normalized χ^2 (which equals one for an ideal fit) improves from 3.5 (old microwindow set) to 1.9 (new microwindow set) for the analysis of O₃ in sunrise 47 of ATLAS-3 (un-

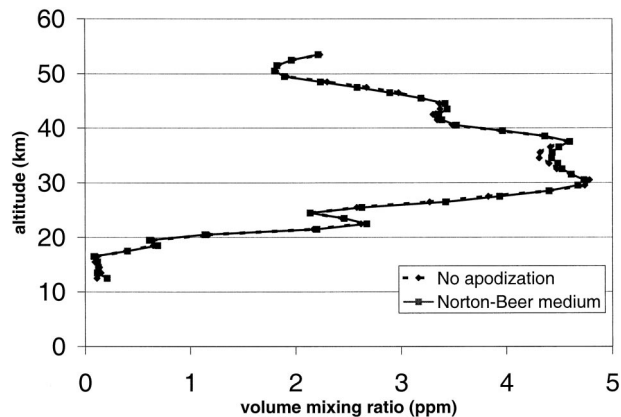


Fig. 6. O₃ retrieval with and without apodization by use of the new microwindow set, ATLAS-3, sunrise 47. Error bars are not shown. Agreement between the two results is generally better than was observed with the old microwindow set. ppm, parts per million.

certainty on each point taken as 1/70 transmittance units). For Norton–Beer medium apodization, the normalized χ^2 improves from 1.9 to 0.73.

Note that the much lower χ^2 from the fitted apodized spectra does not necessarily imply a better fit. It is a numerical artifact resulting from the fact that apodization applies a smoothing to the original data. This smoothing gives much smaller residuals in Fig. 5 than in Fig. 4, for example, yet the results in these two figures are quite comparable in terms of percentage error on the signal peak depths. Consider the extreme case in which apodization flattened everything to a straight line: χ^2 would go to zero, but the spectral information would be completely lost.

5. Discussion

Results for apodized and unapodized spectra showed good agreement within the uncertainties. It is, of course, dangerous to draw conclusions based on the differences between two curves when the error bars overlap (or almost overlap), but when these differences exhibit the same systematic behavior for different molecules and different occultations, you can perhaps credit them as real. On that basis, it was observed that apodization enhanced the oscillatory behavior in the results (when the effect of apodization on the covariance matrix is not taken into account).

Discrepancies for O₃ shown and discussed here did not really exhibit systematic behavior. The discrepancy was generally near (in altitude) the VMR profile peak, but there was no trend to the discrepancies; for some occultations, the unapodized results from the old microwindow set were closer to the results from the new microwindow set, whereas for other occultations the apodized results were closer. This seemed indicative of noise effects, a large random variability to the results arising from having too few microwindows at the important altitudes. The fix applied by a new microwindow set was likely merely a matter of an increased number of microwindows in this altitude region to average out the noise effects.

Failure to account for the effect of apodization on the covariance matrix could be the origin of the systematic (i.e., enhanced oscillatory) discrepancies. Analyzing unapodized spectra seems to dampen out unphysical oscillations in the VMR profiles, but does not remove them entirely. There is an inherent instability associated with the dividing of the atmosphere into a discrete grid for calculations,¹⁸ as is done in the ACE software, but the unphysical oscillations may also indicate the presence of correlations in the unapodized spectra. Under ideal conditions, points in unapodized spectra are statistically independent,⁷ and use of a diagonal covariance for the observations is justified. However, if any corrections are applied to the spectra (e.g., to account for detector nonlinearities, self-apodization from field-of-view effects), correlations between spectral points are introduced, and a diagonal covariance matrix is no longer appropriate. Thus, to be rigorous, an accurate retrieval should carefully track the covariance matrix arising from the transformation from interferogram to spectrum even in the unapodized case. This is not currently implemented in the ACE software, but it is under development.

6. Conclusions

VMR profiles retrieved from apodized and unapodized ATMOS spectra were found to be statistically consistent even when the effect of apodization on the covariance matrix is ignored. Thus the common approach of ignoring this effect to simplify and speed up the processing seems justified. Minor discrepancies can occur when the weak lines are fitted, whereas there is generally little difference in the results when strong lines are fitted. Unphysical oscillatory behavior in the VMR profiles is reduced when the apodized spectra are fitted.

The new set of ozone microwindows reported here reduced the susceptibility to apodization effects for that molecule. Microwindows for other molecules of interest to the ACE mission are under review and will be adjusted to avoid (as much as possible) use of weak lines.

The loss of spectral resolution make the benefits of apodization somewhat dubious. Apodization should be used only if it solves some technical problem.

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