Spectral Deconvolution algorithm
Technical memo

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In this technical memo we presume that the reader has a copy of the original defining papers in hand and accordingly describe changes from the algorithm described in those papers (O'Neill et al., 2001 and O'Neill et al., 2003). The history of the algorithm[1] in terms of Matlab program version numbers, is described below.

Version 4.0

Problems to be resolved

A problem with the Version 3.0 MOE algorithm was an over sensitivity to the estimated error bars in α_f (and in consequence η, τ_f and τ_c). It will be recalled that, in the MOE algorithm, the estimated error bars in α_f were employed to achieve a smooth transition in the forcing condition ($\eta \leq 1$). However it became apparent when processing large AOD smoke data over the Mongu site (Tom Eck) that this (a) created a situation where η values rarely got close to unity because the stochastic error estimates are typically quite large and (b) induced a ceiling effect in η and consequently a strong correlation was created between τ_f and τ_c (which wasn't a problem before the MOE type of error bar forcing). Figure 1 shows a particularily illustrative example of this effect in the Mongu data of 2004.

A second more minor problem was that the empirically developed stochastic expression for the rms error in α' was found to be more complicated than was merited (a much simpler expression was found to reproduce, about equally well, the empirical results of the stochastic simulations of the processing of an ensemble of noisy AOD spectra). This new rms expression was;

$$\Delta\alpha' = 10\ \sigma(\tau_a)/\tau_a$$

where $\sigma(\tau_a)$ is the rms error in the polynomial-fitted AOD.

[1] written originally as a Matlab program called tauf_tauc.m, but, for example, converted to C++ for AERONET

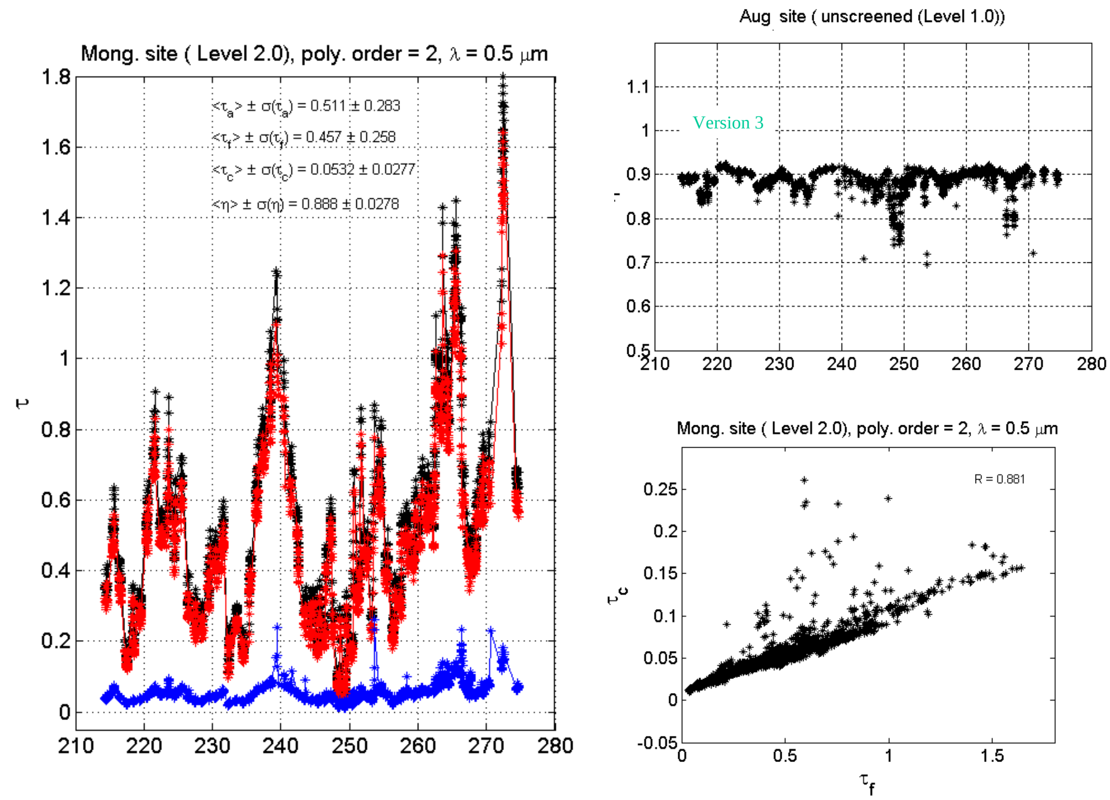

Figure 1 - Artificial correlation between τ_c and τ_f and ceiling effect in η induced by the Version 3.0 (MOE) physical forcing when η is near unity.

Resolution of Version 3.0 problems in Version 4.0

A more general representation of the type of weighted averaging which occurs when $\eta \rightarrow 1$ (which includes the MOE) case is[2];

$\alpha_f(\alpha_f^{(1)}) = \omega(\alpha_f^{(1)}) \alpha + [1 - \omega(\alpha_f^{(1)})] (\alpha_f^{(1)} + \Delta\alpha_f)$

where $\alpha_f^{(1)}$ is the uncorrected estimate of α_f, $\alpha_f(\alpha_f^{(1)})$ is the corrected estimate, $\omega(\alpha_f^{(1)})$ is a weighting function and $\Delta\alpha_f$ is the estimated rms error in α_f. The pragmatic approach to eliminating the problem discussed above is to weight the recomputed α_f mean more towards α (towards $\eta = 1$) than $\alpha f^{(1)} + \Delta\alpha_f$ rather than a straight unweighted mean between the same two quantities as was done for the MOE (Mean of Extrema approach) method of Versions 2 and 3 (and the same idea for the $\eta = 0$ forcing). This means $\omega(\alpha_f^{(1)}) > 0.5$ (where $\omega(\alpha_f^{(1)}) = 0.5$ for the MOE approach). The justification is that the part of the normal curve below $\alpha_f^{(1)} = \alpha$ should have some influence on the corrected α_f value (as opposed to none at all in the MOE). The details of this correction in terms of the analytical development of the quadratic expression for $\omega(\alpha_f^{(1)}) = b_0 + b_1\alpha_f^{(1)} + b_2[\alpha_f^{(1)}]^2$ and the 3rd order expression for $\alpha_f(\alpha_f^{(1)})$ are available from Norm O'Neill. Figure 2 shows how the effects of correlation between τ_c and τ_f and the ceiling effect in η is significantly reduced with the application of the Version 4.0 algorithm. This result is very similar to turning physical forcing off (without the infringements of the $\eta = [0, 1]$ limits which plague the case of no physical forcing); in other words, virtually no new correlation is induced by the algorithm. The residual correlation could well be real (coarse mode smoke being generated at the same time as fine mode smoke particles).

Figure 3 shows a schematic of the Version 3.0 and Version 4.0 averaging schemes.

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[2] a similar approach was taken when $\eta \rightarrow 0$

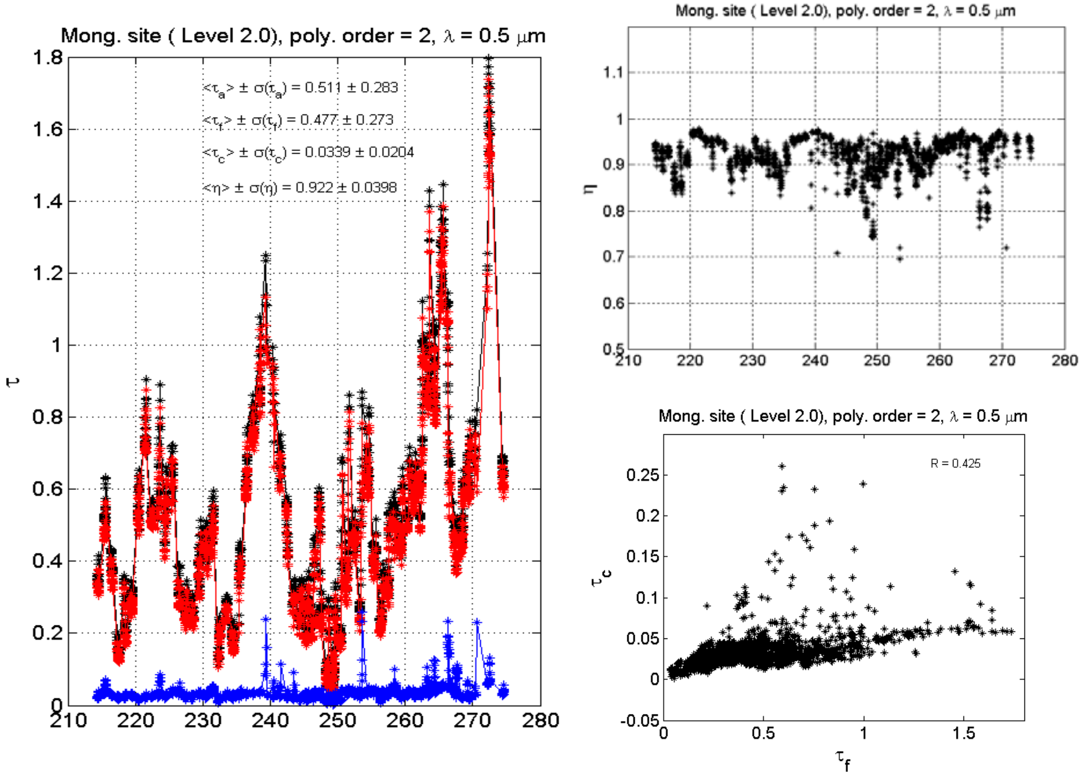

Figure 2 - Significantly reduced correlation between τ_c and τ_f using Version 4.0 algorithm.

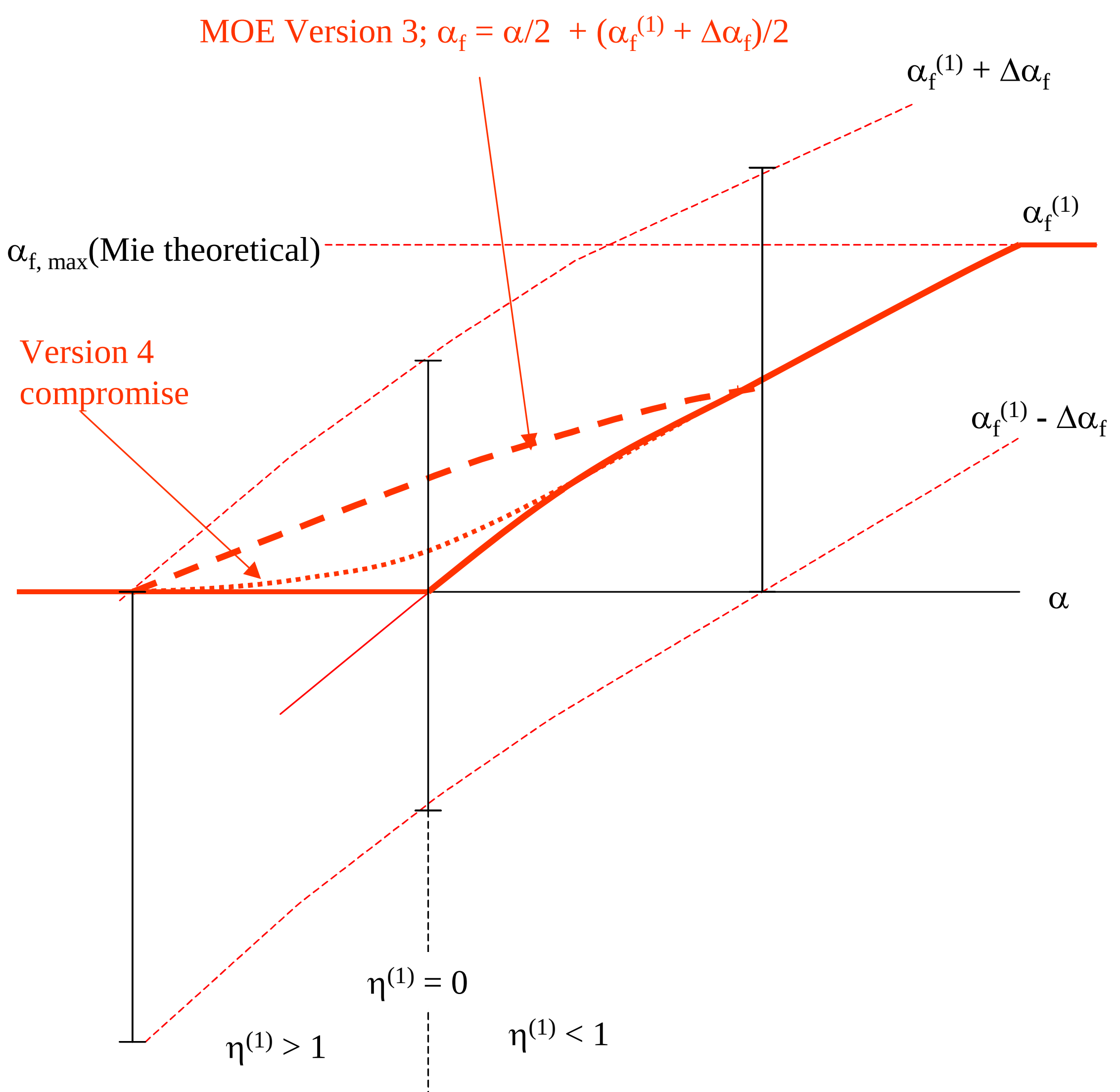

Figure 3 - Conceptual physical forcing illustration for the Version 3 and Version 4 algorithms. The solid vertical lines are the error bars in α_f. The dotted red line is the Version 3.0 (MOE) solution while the dashed bold red line is the Version 4.0 (quadratic weighting) solution. The superscript (1) refers to the uncorrected solution. The bold solid red line is the brute force correction without any error smoothing while (non-bold) solid red line (mostly hidden by the bold solid red line) is the uncorrected solution

Version 3.0

In March of 2005 Version 3.0 of tauf_tauc.m, to be implemented in the new AERONET processing system (called Version 2.0) was delivered. The problems which motivated a new version and the solutions effected are detailed below.

Problems to be resolved in Version 2.0

(i) Version 2.0 still produced anomalous values for very large input AOD errors (discovered when the algorithm was applied to airborne AOD data which had nominal AOD errors >> nominal CIMEL AOD errors) : for very large AOD errors the "mean of extrema correction" was appropriately limited at the lower bound but there simply was no analogous upper bound when the uncertainty limits of α_f were up in the stratosphere (induced by overly large AOD errors) and thus the corrected value of α_f was excessively large (and in consequence the η values were too small).

(ii) The $\alpha_f' = f(\alpha_f)$ polynomial was moderately biased because it didn't include sufficiently small fine-mode PSD standard deviation cases in its envelope of uncertainty and because the original relationship (equation (7) of *O'Neill et al.* [2001]) was not wavelength dependent when clearly it should be.

Resolution of Version 2.0 problems in Version 3.0

Version 3.0 of the spectral deconvolution algorithm was different from the Sept. 8 (Version 2.0) algorithm in the following ways ;

(i) physical forcing was rendered "symmetrical" in Version 3.0 by applying it to the upper as well as the lower physical bounds of α_f (the upper bounds, $\alpha_{f,max,\ theoretical}$ being spectrally dependent and ~ 3.5 as determined by Mie considerations).
(ii) New spectrally dependent coefficients of the parabola in equation (7) of O'Neill et al. [2001] were employed. These are;

$a_{upper} = -.22$, $b_{upper} = 10^{-0.2388}\,\lambda^{1.0275}$, $c_{upper} = 10^{0.2633} * \lambda^{-0.4683}$
$a_{lower} = -.3$, $b_{lower} = .8$, $c_{lower} = .63$
$a = (a_{lower} + a_{upper})/2$, $b = (b_{lower} + b_{upper})/2$ et $c = (c_{lower} + c_{upper})/2$

where the indices "upper" and "lower" refer to the uncertainties in the coefficients (due to uncertainty in the actual fine mode model). The new uncertainty in α_f (which propagates into the uncertainty in α_f, η, etc.) follows from these expressions, viz;

$$\Delta\alpha'_f = (a_{upper} - a_{lower})/2\ \alpha_f^2 + (b_{upper} - b_{lower})/2\ \alpha_f + (c_{upper} - c_{lower})/2.$$

Remaining problem in Version 3.0

The version 3.0 algorithm does not account for rare cases where $\alpha > \alpha_{f,max,\ theoretical}$ (usually associated with a serious artifact in one of the AOD channels). The solution would mean forcing α to be = $\alpha_{f,max,\ theoretical}$. Rather than changing measurement values (up to this point only inverted values have been modified) it was decided to simply accept the infrequent occurence of this situation (for which $\eta > 1$).

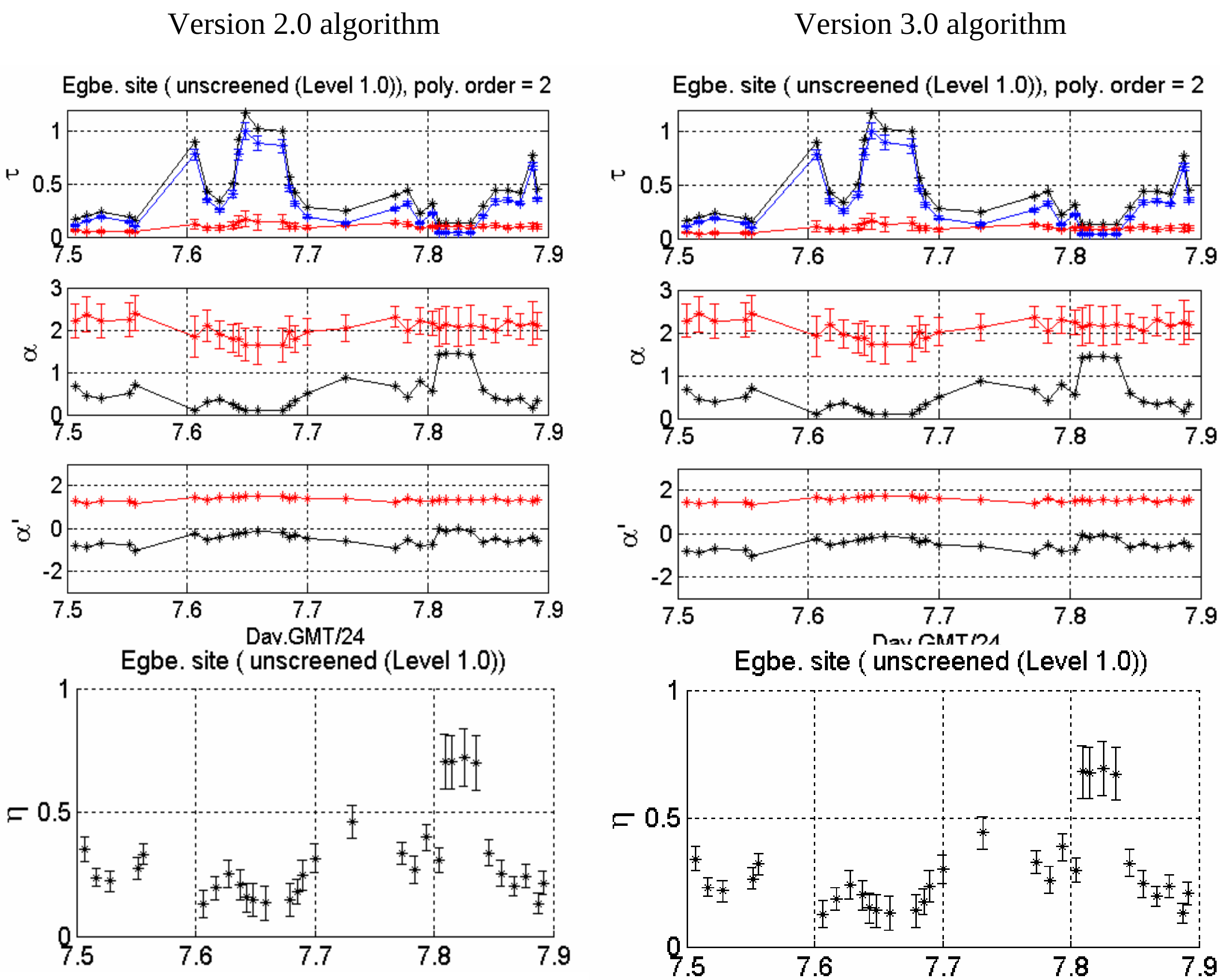

Figure 4 - Version 2.0 and version 3.0 spectral deconvolution results for Egbert, Ontario, Canada (λ = 500 nm). These results are for the same input data employed to produce Figure 4 of *O'Neill et al*. [2003].

Some comparative results

Figure 4 above shows a comparison between Version 2.0 and Version 3.0 results. In this case the changes are very small (as they are also relative to Version 1.0 results shown in Figure 4 of *O'Neill et al*. [2003]). Figure 5 below also shows a case with only very small changes between the algorithms.

Version 2.0 algorithm

Version 3.0 algorithm

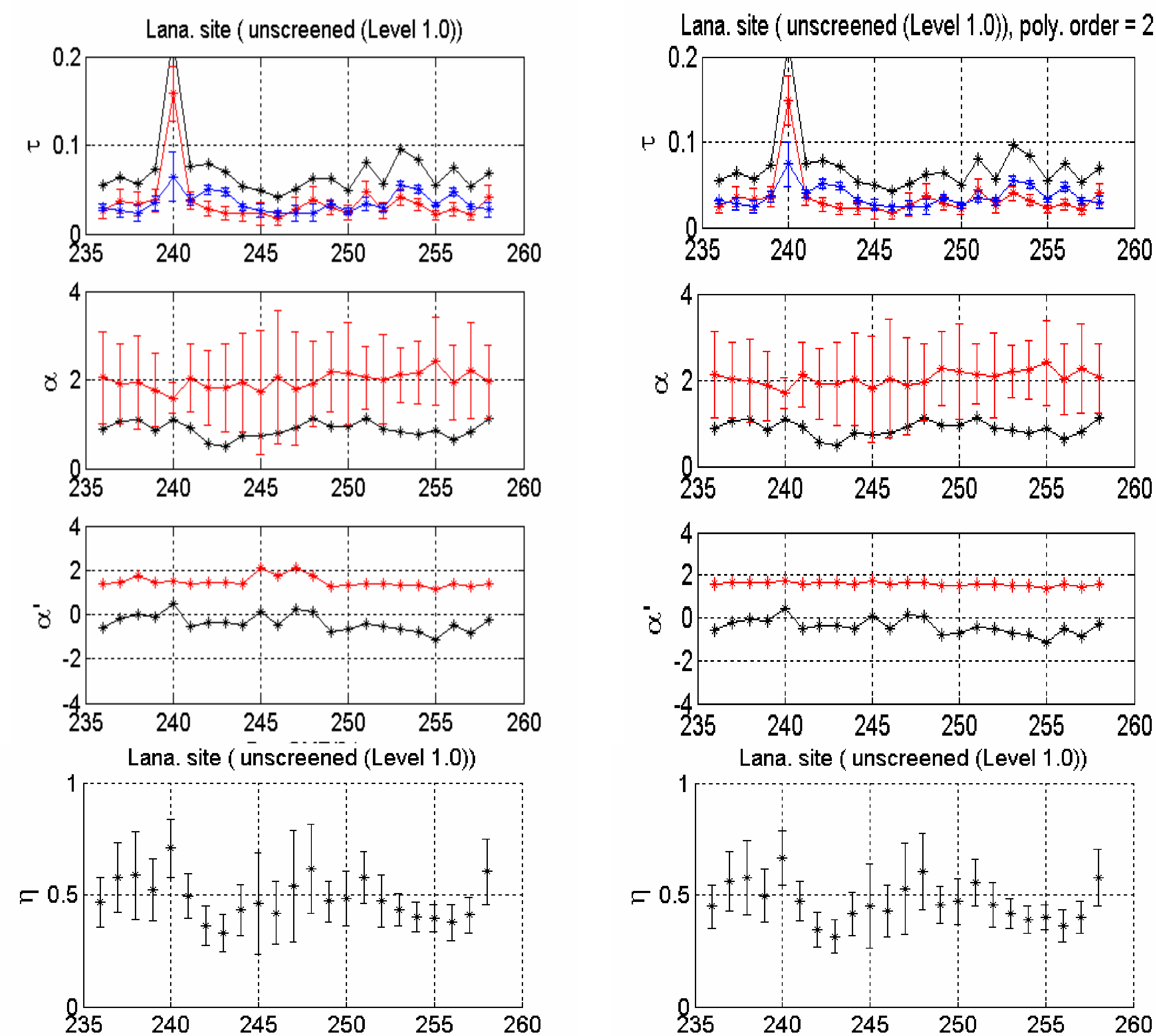

Figure 5 - Version 2.0 and version 3.0 spectral deconvolution results for the Lanai, Hawaii, site, Aug.-Sep 2001, λ = 550 nm (daily averages).

Figure 6 below shows a case where there are slightly more significant changes between the algorithms. Comparison with the Version 1.0 results of Figure 8 in *O'Neill et al*. [2003]) show that the anamolous AOD and Angstrom results of that figure (where $\tau_f > \tau_a$ and $\alpha_f < \alpha$) have appropriately disappeared. The modelled stochastic errors increase moderately from Version 2.0 to Version 3.0 while the nominal α_f and η values decrease and increase respectively by a small amount. Both versions demonstrate the progressively larger errors which one obtains as α_f decreases towards unity (as one approaches large fine mode particles).

Version 2.0 algorithm

Version 3.0 algorithm

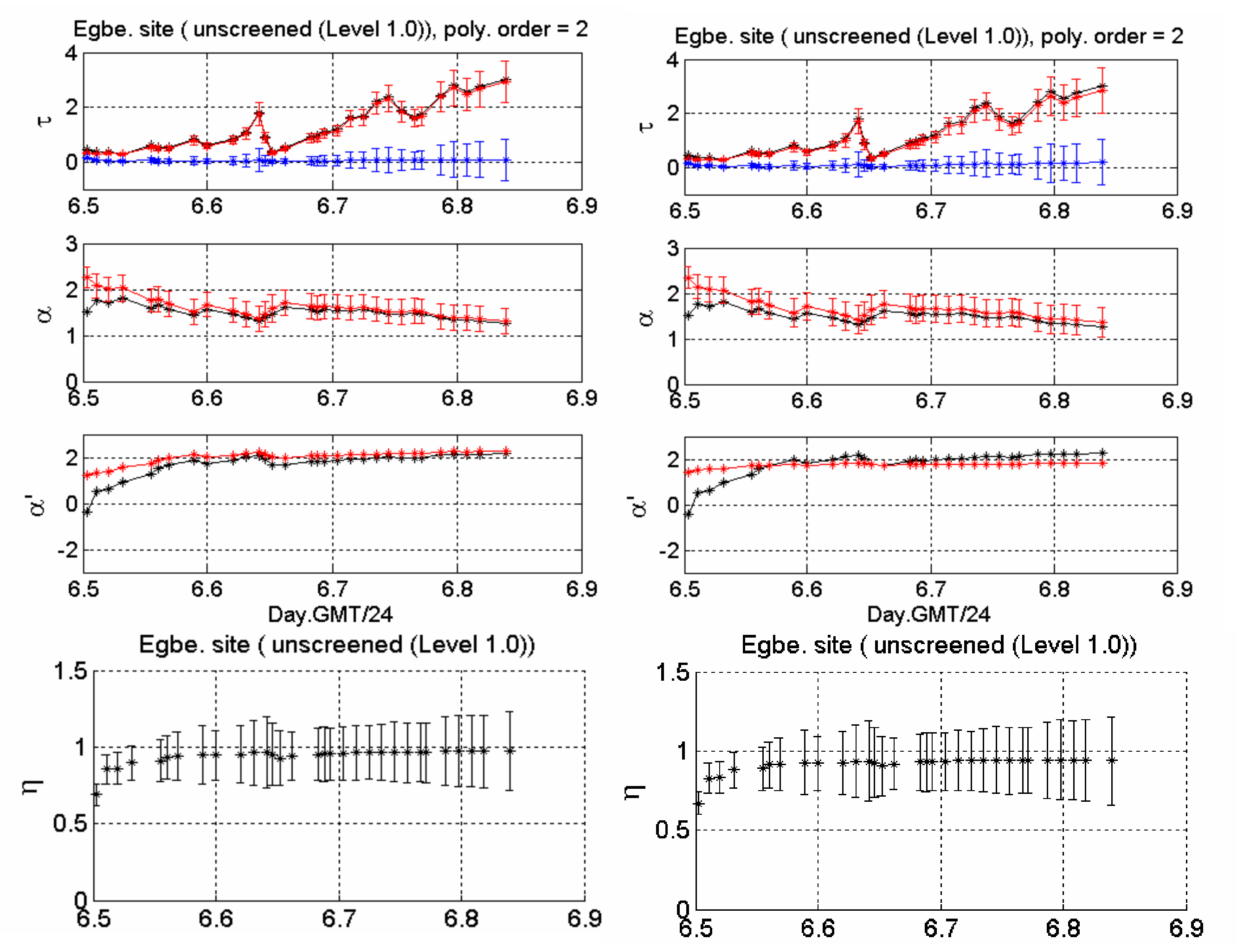

Figure 6 - Version 2.0 and version 3.0 spectral deconvolution results during the first day of the Québec smoke event of July 2002 at Egbert, Ontario, Canada (λ = 500 nm). These results are for the same input data employed to produce Figure 8 of *O'Neill et al*. [2003].

It was found that only extreme cases had any significant effect re the limit of $\alpha_{f,\, max,\, theoretical}$ on α_f. Figure 7 shows Version 2.0 versus 3.0 results for a case of very large AOD input error (precisely when one has problems with extremely large α_f values induced by very large uncertainty bars). It can be seen that the Version 3.0 α_f values are much more stable (which is in itself a positive thing) but that η values do not change by a lot except when the errors in α_f are quite exessive (measurements 1, 16, and 17 which are associated with anamolous artifacts in certain bands).

Version 2.0 algorithm | Version 3.0 algorithm

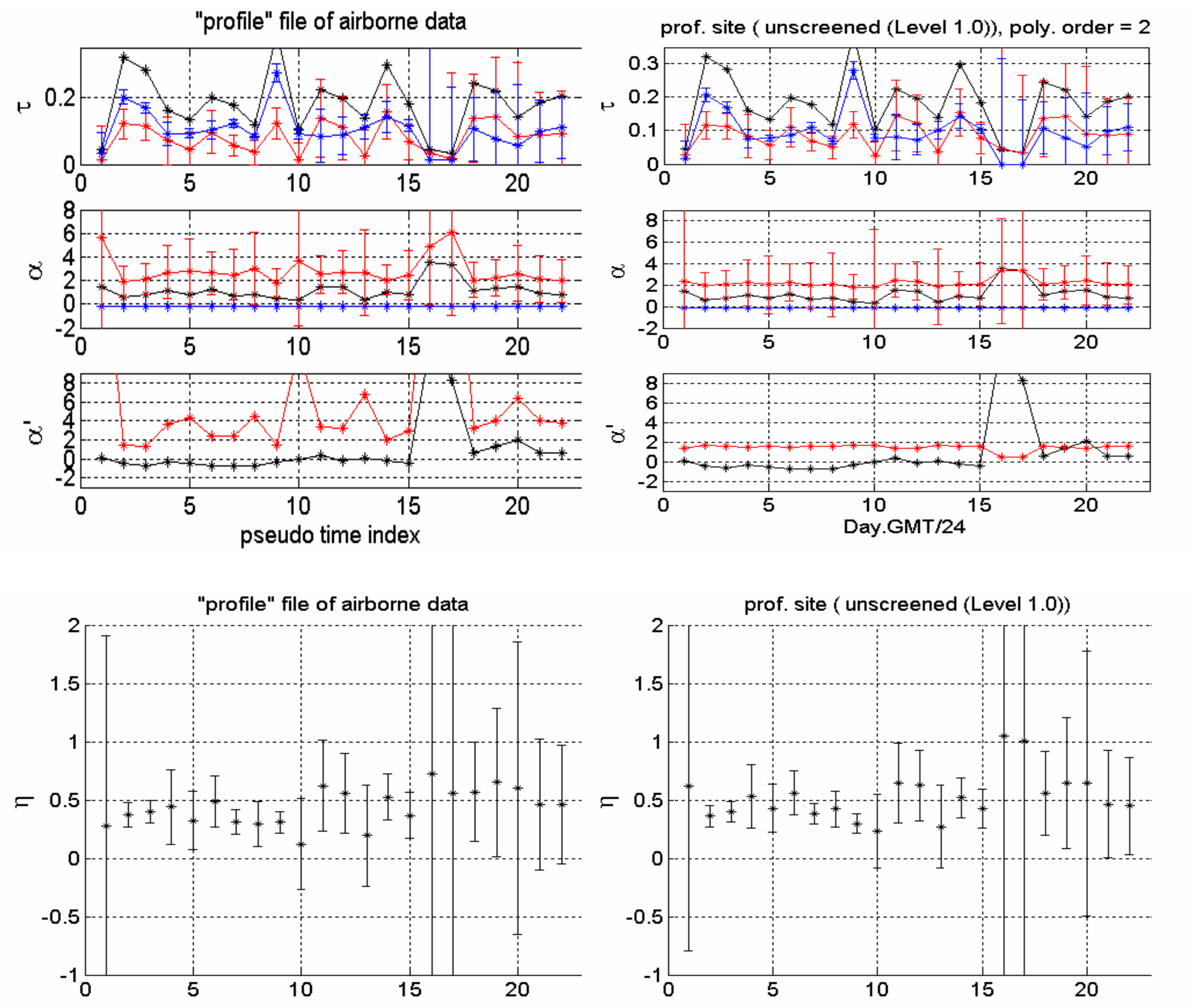

Figure 7 - Version 2.0 and version 3.0 spectral deconvolution results for some airborne data provided by Santiago Grasso. The nominal input AOD error is = 0.039 at a wavelength of λ = 0.55 μm. The x axis represents a measurement # index.

QA issues for Version 3.0

Data processing protocols typically include two or more levels which range from raw data to averaged value-added products. One could view the QA issue in the case of the spectral deconvolution algorithm as a choice between dynamic QA (where no points are eliminated but an error estimate is given for all points) and "pass / no-pass" type of filtering such as cloud screening. Below are some thoughts on each type.

Dynamic QA

The algorithm should be applied to level 1.0, 1.5 and 2.0 AOD since it is intended to discriminate coarse mode from fine mode AODs. In a very real sense it "rides" on the AERONET QA already in place; one could certainly speak of level 1.0, 1.5 and 2.0 values of τ_f, τ_c, and η.

Its not clear that a complementary QA process is necessary in the sense of pass/no-pass filter; the algorithm already provides a dynamic esimation of stochastic error ($\Delta\tau_f$, $\Delta\tau_c$, $\Delta\eta$) for every single AOD spectrum. There is not yet an analogue to this in Oleg's inversion processing because there is no provision for a dynamic error estimate of the derived products (and of course its much more complicated to do). As well, the physical forcing modifications of Version 3.0 have eliminated virtually all cases of non-physical values.

Pass / no-pass type of QA filter

If it is deemed essential to have pass / no-pass type of QA filter then possible candidates would be a combination of the two conditions below. The filter thresholds selected below represent a fairly liberal constraint while ensuring that extreme anomolies are eliminated.

- a threshold on the estimated stochastic error in $\Delta\tau_f$, $\Delta\tau_c$, $\Delta\eta$ ($\Delta\eta < 0.5$ would be a reasonable choice)
- some threshold on the AOD polynomial regression error $\Delta\tau_a / \tau_a$ (an indicator of how distorted the AOD spectrum is). $\Delta\tau_a / \tau_a < 0.3$ would be a liberal choice.

Relationship with Dubovic inversion outputs

The differences between the spectral deconvolution algorithm and the fine-mode / coarse-mode optical depths from the Dubovik inversion are not an issue since the current Dubovik output is the equivalent of what the community calls SMF (sub-micron fraction) as opposed to the spectral deconvolution algorithm output which is essentially an FMF (fine mode fraction) type of discrimination[3]. The former is a purely mechanical cutoff in radius (which is fundamentally how mechanical discriminators work) while the latter is a total mode discrimination (arguably more physically fundamental in that the different modes represent different physical origins). This means that $\tau_{c, SM} < \tau_{c, FM}$ so that $\tau_{f, SM} > \tau_{f, FM}$ and hence SMF > FMF ($\eta_{SM} > \eta_{FM}$). The new Dubovik inversion which will base the fine-mode / coarse-mode division on the minimum value of the (volume) particle size distribution value rather than the current 0.6 μm cutoff will be more analogous to a FMF type of division.

Version 2.0

On or about Sept. 8, 2004 a new tauf_tauc.m version with a "physical_forcing" option for eliminating $\eta > 1$ problems was delivered to AERONET. Details are given below.

Problems resolved with respect to the Version 1.0 algorithm

Under certain conditions the value of the ("monochromatic") Angstrom exponent (α) exceeded the maximum value of α_f permitted by equation (7) of O'Neill et al., (2001). This automatically created a non-physical situation where the fine mode fraction (η) was greater than unity (and the spectral derivative α' was as a consequence greater than α_f'). These conditions usually corresponded to cases of thick, aged (large particle) smoke when α' was large and α was small. The problem was fixed in a smoothly varying fashion by implementing the "physical forcing" option described in the section immediately below.

Resolution of Version 1.0 problems in Version 2.0

If any portion of the uncertainty bar of α_f (computed from the stochastic error estimate described in O'Neill et al., 2001) was lower than α then a new value of α_f was computed as the mean of the upper extrema of the estimated α_f uncertainty and α. This "mean of extrema" (MOE) modification is represented by the dotted line in Figure 3.

Version 1.0

This is basically the algorithm described in O'Neill et al., 2001 and O'Neill et al., 2003 and it was the first algorithm delivered to AERONET (to Ilya Slutsker).

References

1. O'Neill, N. T., Dubovik, O., Eck, T. F., A modified Angstrom coefficient for the characterization of sub-micron aerosols, *App. Opt.*, Vol. 40, No. 15, pp. 2368-2374, 2001.

[3] the spectral deconvolution approach is really spectral in nature (one assumes apriori properties of the coarse mode spectrum). This spectral approach is much more closely tied with the FMF than the SMF. In terms of the notation in O'Neill et al. (2003), FMF = η.

2. O'Neill, N. T.,T. F., Eck, A. Smirnov, B. N.Holben, S. Thulasiraman, Spectral discrimination of coarse and fine mode optical depth, Vol.. 108, *J. Geophys. Res.,* No. D17, 4559-4573, 10.1029/2002JD002975, 2003.