Supplemental to:

The New MISR Research Aerosol Retrieval Algorithm: A Multi-Angle, Multi-Spectral, Bounded-Variable Least Squares Retrieval of Aerosol Particle Properties over Both Land and Water

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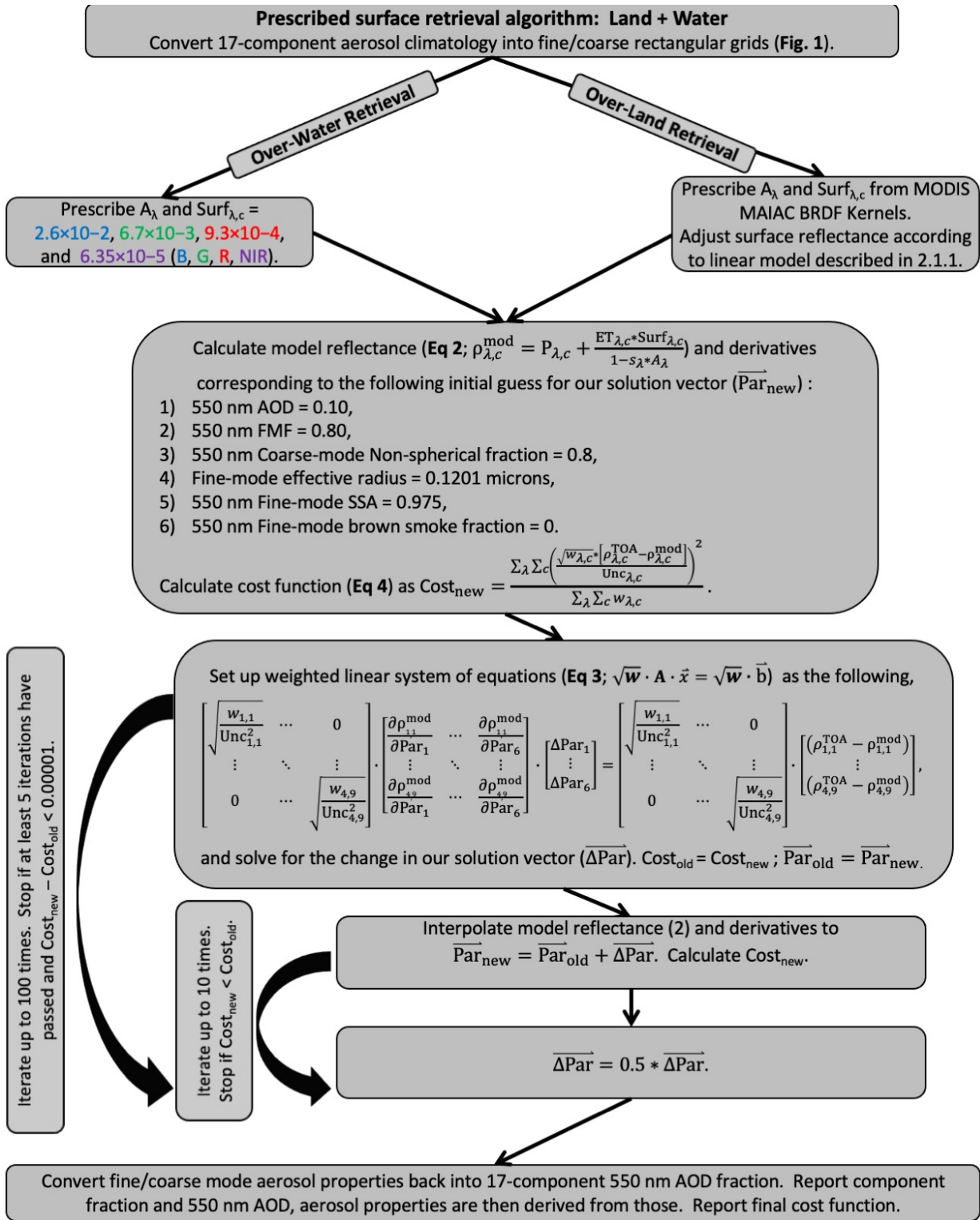*Correspondence to*: James A. Limbacher (James.Limbacher@nasa.gov)

Prescribed surface retrieval algorithm: Land + Water
Convert 17-component aerosol climatology into fine/coarse rectangular grids (**Fig. 1**).

Over-Water Retrieval

Over-Land Retrieval

Prescribe A_λ and $\text{Surf}_{\lambda,c}$ =
$2.6\times10{-2}$, $6.7\times10{-3}$, $9.3\times10{-4}$, and $6.35\times10{-5}$ (B, G, R, NIR).

Prescribe A_λ and $\text{Surf}_{\lambda,c}$ from MODIS MAIAC BRDF Kernels.
Adjust surface reflectance according to linear model described in 2.1.1.

Calculate model reflectance (**Eq 2**; $\rho_{\lambda,c}^{\text{mod}} = P_{\lambda,c} + \frac{ET_{\lambda,c}*\text{Surf}_{\lambda,c}}{1-s_\lambda*A_\lambda}$) and derivatives corresponding to the following initial guess for our solution vector ($\overrightarrow{\text{Par}}_{\text{new}}$) :

1) 550 nm AOD = 0.10,
2) 550 nm FMF = 0.80,
3) 550 nm Coarse-mode Non-spherical fraction = 0.8,
4) Fine-mode effective radius = 0.1201 microns,
5) 550 nm Fine-mode SSA = 0.975,
6) 550 nm Fine-mode brown smoke fraction = 0.

Calculate cost function (**Eq 4**) as $\text{Cost}_{\text{new}} = \dfrac{\sum_\lambda \sum_c \left(\frac{\sqrt{w_{\lambda,c}}*\left[\rho_{\lambda,c}^{\text{TOA}}-\rho_{\lambda,c}^{\text{mod}}\right]}{\text{Unc}_{\lambda,c}}\right)^2}{\sum_\lambda \sum_c w_{\lambda,c}}$.

Set up weighted linear system of equations (**Eq 3**; $\sqrt{w} \cdot A \cdot \vec{x} = \sqrt{w} \cdot \vec{b}$) as the following,

$$\begin{bmatrix} \sqrt{\frac{w_{1,1}}{\text{Unc}_{1,1}^2}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\frac{w_{4,9}}{\text{Unc}_{4,9}^2}} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial\rho_{1,1}^{\text{mod}}}{\partial\text{Par}_1} & \cdots & \frac{\partial\rho_{1,1}^{\text{mod}}}{\partial\text{Par}_6} \\ \vdots & \ddots & \vdots \\ \frac{\partial\rho_{4,9}^{\text{mod}}}{\partial\text{Par}_1} & \cdots & \frac{\partial\rho_{4,9}^{\text{mod}}}{\partial\text{Par}_6} \end{bmatrix} \cdot \begin{bmatrix} \Delta\text{Par}_1 \\ \vdots \\ \Delta\text{Par}_6 \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{w_{1,1}}{\text{Unc}_{1,1}^2}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\frac{w_{4,9}}{\text{Unc}_{4,9}^2}} \end{bmatrix} \cdot \begin{bmatrix} (\rho_{1,1}^{\text{TOA}} - \rho_{1,1}^{\text{mod}}) \\ \vdots \\ (\rho_{4,9}^{\text{TOA}} - \rho_{4,9}^{\text{mod}}) \end{bmatrix},$$

and solve for the change in our solution vector ($\overrightarrow{\Delta\text{Par}}$). $\text{Cost}_{\text{old}} = \text{Cost}_{\text{new}}$; $\overrightarrow{\text{Par}}_{\text{old}} = \overrightarrow{\text{Par}}_{\text{new}}$.

Iterate up to 100 times. Stop if at least 5 iterations have passed and $\text{Cost}_{\text{new}} - \text{Cost}_{\text{old}} < 0.00001$.

Iterate up to 10 times. Stop if $\text{Cost}_{\text{new}} < \text{Cost}_{\text{old}}$.

Interpolate model reflectance (2) and derivatives to $\overrightarrow{\text{Par}}_{\text{new}} = \overrightarrow{\text{Par}}_{\text{old}} + \overrightarrow{\Delta\text{Par}}$. Calculate Cost_{new}.

$\overrightarrow{\Delta\text{Par}} = 0.5 * \overrightarrow{\Delta\text{Par}}.$

Convert fine/coarse mode aerosol properties back into 17-component 550 nm AOD fraction. Report component fraction and 550 nm AOD, aerosol properties are then derived from those. Report final cost function.

Figure S1) Flow chart of the MISR RA prescribed surface aerosol retrieval.

Retrieved surface retrieval algorithm: Land + Water
Convert 17-component aerosol climatology into 65 discrete aerosol mixtures (described in 2.1.2).

Over-Water → **Water Surface Retrieval**
Store surface properties and residuals for every aerosol mixture

Loop over every AOD found in LUT (Table 2).

Over-Land → **Land Surface Retrieval**
Store surface properties and residuals for every aerosol mixture

AOD Bisection iteration:
Use 6 AOD bisections to iterate towards optimum AOD and surface properties for all 65 aerosol mixtures.
Calculate **cost function** with optimum AOD and surface properties (A_λ^* and L_c) for each aerosol mixture using **Eq 6**.

Mixture and surface property aggregation:
Convert cost function to exponential **mixture weights (MW$_m$)** via **Eq 9**.
Calculate aggregate aerosol component fractions (Table 1), cost, and surface properties using mixture weights.
Calculate effective A_λ by accounting for multiple reflections using the aggregate atmospheric backscatter (s_λ) and A_λ^*.

Water Surface Retrieval:
L_c=1.0 (Lambertian surface)

Solve A_λ^* (Eq 7) setting L_c=1 (Lambertian),

$$A_\lambda^* = \frac{\sum_c \frac{w_{\lambda,c}}{Unc_{\lambda,c}^2} * ET_{\lambda,c} * L_c * \left[\rho_{\lambda,c}^{TOA} - P_{\lambda,c}\right]}{\sum_c \frac{w_{\lambda,c}}{Unc_{\lambda,c}^2} * \left[L_c * ET_{\lambda,c}\right]^2}.$$

Constrain A_λ^*, according to (applied in order):
A_B^* =max(0.005, min(A_B^*, 0.35)),
A_G^* =max(0.003, min(A_G^*, 0.35)),
A_R^* =max(5E^{-4}, min(A_R^*, 0.35)),
A_N^* =max(8E^{-5}, min(A_N^*, 0.2)),
A_N^* =Min(0.9 * A_B^*, 0.9* A_G^*, 0.9* A_R^*, A_N^*).

Cost function (Eq 6):

$$\sum_\lambda \sum_c \frac{\left(\frac{\sqrt{w_{\lambda,c}} * \left[\rho_{\lambda,c}^{TOA} - \left(P_{\lambda,c} + ET_{\lambda,c} * A_\lambda^* * L_c\right)\right]}{Unc_{\lambda,c}}\right)^2}{\sum_\lambda \sum_c w_{\lambda,c}}$$

Mixture Weights (Eq 9):

$$MW_m = \frac{\exp\left(\frac{Cost_{min} - Cost_m}{Cost_{min} + 0.01}\right)}{\sum_m \left[\exp\left(\frac{Cost_{min} - Cost_m}{Cost_{min} + 0.01}\right)\right]}$$

Iterate 2x to optimize initial A_λ^* and L_c.

Land Surface Retrieval:
L_c=1.0 (Initially assume Lambertian surface)

Solve A_λ^* (Eq 7) using assumed/refined L_c,

$$A_\lambda^* = \frac{\sum_c \frac{w_{\lambda,c}}{Unc_{\lambda,c}^2} * ET_{\lambda,c} * L_c * \left[\rho_{\lambda,c}^{TOA} - P_{\lambda,c}\right]}{\sum_c \frac{w_{\lambda,c}}{Unc_{\lambda,c}^2} * \left[L_c * ET_{\lambda,c}\right]^2}.$$

Constrain A_λ^*, according to (applied in order):
A_B^* =max(0.015, min(A_B^*, 0.4)),
A_G^* =max(0.02, min(A_G^*, 0.5)) ,
A_R^* =max(0.025, min(A_R^*, 0.6)),
A_N^* =max(0.05, min(A_N^*, 0.7)),
A_B^*=min(A_B^*, A_N^*),
A_B^*=min(A_B^*,A_R^*),
A_B^* =max(A_B^*, 0.2*A_N^*),
A_G^*=max(A_G^*,0.3*A_N^*),
A_R^*=max(A_R^*, 0.4*A_N^*),
A_N^*=max(A_λ^*).

Refine L_c (Eq 8) using constrained A_λ^*,

$$L_c = \frac{\sum_\lambda \frac{w_{\lambda,c}}{Unc_{\lambda,c}^2} * A_\lambda^* * ET_{\lambda,c} * \left[\rho_{\lambda,c}^{TOA} - P_{\lambda,c}\right]}{\sum_\lambda \frac{w_{\lambda,c}}{Unc_{\lambda,c}^2} * \left[A_\lambda^* * ET_{\lambda,c}\right]^2},$$

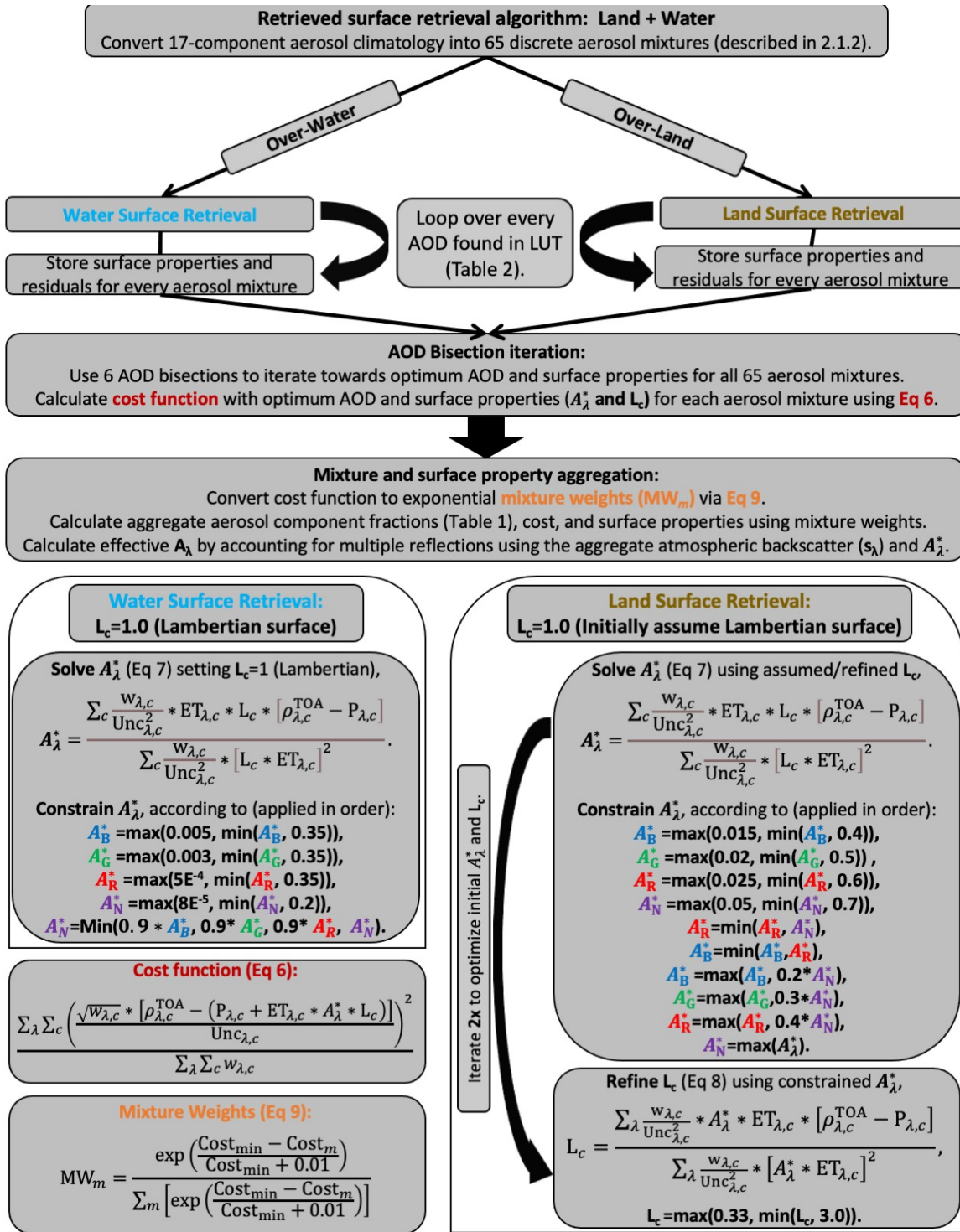L_c =max(0.33, min(L_c, 3.0)).

Figure S2) Flow chart of the MISR RA retrieved surface aerosol retrieval. Note the panel titled "Surface Retrieval Iteration", which is referenced twice in the flow chart, and explains how surface reflectance is retrieved over both land and water.