Cover letter

To

Dr. Sylwester Arabas
Topic Editor,
Geoscientific Model Development (GMD)

15 May 2024

Subject: Final author reply to the editor.
Manuscript Title: AeroMix v1.0.1: a Python package for modeling aerosol optical properties and mixing states.
Manuscript ID: EGUSPHERE-2024-62

Dear Dr. Sylwester Arabas,

Along with this letter, we submit the revised version of our manuscript titled "AeroMix v1.0.1: A Python package for modeling aerosol optical properties and mixing states" to the Journal of Geoscientific Model Development (GMD).

The co-authors and I appreciate the constructive comments on this manuscript by the reviewers. The comments have been very thorough and valuable in improving the manuscript. We have taken them fully into account while revising the manuscript. Our detailed responses to the comments are attached, with line numbers referenced as they appear in the tracked changed version.

All the authors agreed with the revision of this manuscript.

I request you to kindly take the necessary steps for the manuscript's earliest review.

Thank you.

Sincerely yours,

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Response notes

General comments

The study fits into the scope of GMD. Minor organization of the methods section is needed as described below.

Reply: We appreciate and thank the reviewer's valuable and detailed comments and recommendation. All comments have been taken into account, as described below.

Introduction

1. When discussing motivation, the mixing state of aged aerosol (far from source) is important for CCN (Farmer, Cappa, and Kreidenweis 2015). McFiggans et al. 2006 is another source discussing CCN from close to source and aged populations.

    Reply: As per your suggestion the text is revised as (Page #2, Line #33).

    "Knowledge of the size-resolved aerosol chemical composition, size distribution, and mixing state is required to predict cloud condensation nuclei (CCN) concentrations for freshly emitted and aged aerosols (McFiggans et al., 2006; Ervens et al., 2010; Farmer et al., 2015)."

Model Overview

2. For the readers' convenience, add a table for chemical species modeled (IS, WS, BC, SS, MD). Table columns should include the name, shorthand name (e.g. IS), species considered/represented (IS includes soil dust, fly ash, and non-hygroscopic organic matter from biomass burning), and modes present (nucleation (nm), accumulation (am), coarse (cm)).

    Reply: A new table presenting the compositions of predefined components, their shorthand name, constituting species, along with their dry state (0% RH) size distribution parameters and refractive index (at 0.5 µm) is added (Page #7). The discussion about constituting species in the lines from #99-107 is removed to avoid redundancy.

Table 1: Size distribution parameters, specific densities, and refractive indices of predefined aerosol components at dry state (0% RH).

Aerosol component	Constituting species	Mode radius (µm)	Standard deviation	specific density (g cm^{-3})	Refractive index at 0.5 µm
Insoluble (IS)	Soil dust, fly ash, and non-hygroscopic organic	0.471	2.51	2.0	$1.53 + 8 \times 10^{-3}i$

	matter.				
Water-soluble (WS)	SO_4^{2-}, NO_3^-, NH_4^+ and hygroscopic fraction of organic matter.	0.0212	2.24	1.8	$1.53 + 5 \times 10^{-3}$i
Black carbon (BC)	Black carbon aerosols	0.0118	2	1.8	$1.75 + 4.5 \times 10^{-1}$i
Sea-salt accumulation mode (SSam)	Sea salt aerosols	0.209	2.03	2.2	$1.5 + 1.55 \times 10^{-8}$i
Sea-salt coarse mode (SSam)		1.75	2.03		
Mineral dust nucleation mode (MDnm)	Desert dust	0.007	1.95	2.6	$1.53 + 7.8 \times 10^{-3}$i
Mineral dust accumulation mode (MDam)		0.39	2		
Mineral dust coarse mode (MDcm)		1.9	2.15		
Stratospheric sulfate (SU)	Sulfate aerosols from volcanic eruption.	0.0695	2.03	1.7	$1.431 + 1 \times 10^{-8}$i

3. It is unclear if the optical properties for coated MD particles are calculated using Mie theory or TMM. Clarify if TMM only applies to particles comprised of 100% MD.

Reply: Optical properties of particles composed solely of MD are calculated using the TMM code. These values are adopted from Koepke et al. (2015). To avoid further confusion, the component names are mentioned explicitly. The lines #119-124 (Pages #5&6) are revised as

"The optical properties of each component, except for MDnm, MDam, and MDcm components, are calculated using the Mie theory (Mie, 1908). This calculation assumes that the particles are spherical in shape and follow a lognormal size distribution. The calculated optical properties are normalized to one particle cm^{-3} and stored, which can then be scaled to any given number concentration. MDnm, MDam, and MDcm components are modeled using the T-Matrix Method (TMM) (Waterman, 1971; Mishchenko et al., 1999) to account for their non-sphericity (Koepke et al., 2015)."

Optical properties of all the core-shell mixed particles are modeled using the coated-sphere Python Mie calculation program PyMieScatt; as indicated in the manuscript (Page #8, Line #149).

4. The exponential function for the vertical profile of aerosol concentration is mentioned in Eq. 5; however, only the cubic function is utilized in the modeling section considering it provides the better fit based on R2 and RMSE values. The authors do not necessarily need to include the exponential function since it is not used to

model vertical profiles in this paper.

Reply: We prefer to retain the exponential function to model the aerosol vertical profile. It is primarily due to the considerations aimed at offering flexibility in the AeroMix model to adopt under different scenarios based on the following considerations:

    a.   The predecessor model, OPAC, uses the exponential function to model the aerosol vertical profile. Retaining this function allows for comparisons between AeroMix-modeled AOD values with OPAC-modeled ones, facilitating consistency in analyses.

    b.   The cubic function is employed for modeling due to its superior fit based on R^2 and RMSE values described in this paper. However, it may not always be applicable in locations lacking aerosol vertical profile measurements. Therefore, selecting suitable generalized exponential functions for the aerosol mixture (e.g., marine, urban, desert, continental) becomes necessary.

    c.   Offering users the option to choose from the given three types of aerosol vertical profiles (exponential, cubic, and homogeneous) enhances flexibility, enabling selection based on the specific study location and layer characteristics.

The lines #179-188 (Page #9) are revised as following to provide more clarity.

"The vertical profile of aerosol concentration in each layer can be modeled as homogenous or as an exponential function given by,

$$N(h) = N(0)exp\left(-h/z\right), \tag{1}$$

where $N(0)$ is the number concentration of aerosol at the layer bottom, h is the height from the layer bottom, and z is the scale height representing the change in aerosol concentration with height (Hess et al., 1998). Standard exponential profiles for different aerosol types provided by Hess et al. (1998) can be utilized for locations lacking aerosol vertical profile measurements. Alternatively, it can be modeled using a cubic function (Eq. (6)) when aerosol vertical profile measurements are available.

$$N(h) = N(0)(ah^3 + bh^2 + ch + d), \tag{2}$$

where a, b, c, and d are the coefficients when $N(0) = 1$ (Russo et al., 2006)."

We hope you will agree that maintaining the exponential function alongside other options to provide users a comprehensive package, ensuring adaptability to diverse research contexts.

5. This section was jumpy and difficult to follow. I suggest further dividing into subsections:

Reply: In accordance with your suggestion, we have carefully divided section 3 into subsections as follows (Pages #10-18, Lines #196-348):

"

3. Modeling aerosol mixing state with AeroMix

The primary objective of AeroMix is to provide an open-source aerosol optical model framework tailored to support inversion algorithms for modeling both aerosol mixing states and their physical and chemical characteristics. The probable aerosol mixing states are modeled with AeroMix using the Mie inversion technique by iteratively comparing the multispectral measurements of aerosol optical properties with modeled ones for different mixing scenarios until they converge within the observational error (Fig. 1) (Chandra et al., 2004; Dey et al., 2008; Kaskaoutis et al., 2011; Ramachandran and Srivastava, 2016; Srivastava et al., 2016, Srivastava et al., 2018).

3.1. Comparison with OPAC

Initially, the AeroMix modeled aerosol properties were compared with OPAC for ten externally mixed cases given in OPAC, namely continental clean, continental average, continental polluted, urban, desert, maritime clean, maritime polluted, maritime tropical, Arctic, and Antarctic. The AeroMix computed aerosol mass concentrations (M_a) of all ten cases, as well as AOD, SSA, and asymmetry parameters, showed excellent agreement ($r = 0.99$, slope = ~ 1) with OPAC-derived ones (Figs. S1 and S2).

3.2. Model setup

3.2.1. Study region and data

AeroMix performance was further assessed by determining the probable aerosol mixing states over two contrasting environments: Kanpur, India (26.513° N, 80.232° E, 123 m AMSL; urban) and the Bay of Bengal (11.99°- 20.61°N, 80.52°-92.55° E; BoB; marine) representing diverse aerosol mixtures. Past endeavors to deduce intricate aerosol mixing states through Mie model inversion were hindered by the OPAC model's constraints on the number of plausible mixing state cases. The efficacy of this method relies on the accuracy of input parameters, encompassing AOD, SSA, aerosol vertical profile, RH, refractive index, size distribution, and mixing state assumptions. Therefore, collocated and concurrent measurements of quality-controlled spectral AODs, spectral SSAs, spectral asymmetry parameter, vertical profile of aerosols, aerosol chemical composition, mixed layer height (MLH), and RH were used for the first time over Kanpur and the BoB; in South Asia to model the probable mixing states of aerosols using AeroMix. These measurements were taken from January 2007 to December 2009 at Kanpur and during the Winter-Integrated Campaign for Aerosols, gases and Radiation Budget (W-ICARB) conducted from December 2008 to January 2009 over the BoB (Moorthy et al., 2010). The seasonal mean MLH and β_{ext} profiles at 532 nm obtained from NASA Micro-Pulse Lidar Network (MPLNET) collected over Kanpur during the period May 2009 – November 2015 are utilized in this study. β_{ext} profiles at 532 nm over the western-BoB (W-BoB) and northern-BoB (N-BoB) are obtained from Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP). A summary of various aerosol and meteorological datasets used in the present study is provided in Table 2. A detailed description of the datasets used can be found in the reference therein and presented in supplementary information (SI). The locations of Kanpur, W-BoB, N-BoB, and the W-ICARB cruise track, along with seasonal average surface wind directions, are presented in Fig. 2.

3.2.2. Mixing state assumptions

The analysis encompasses eight aerosol components (IS, WS, BC, SSam, SScm, MDnm, MDam, and MDcm) in an externally mixed state and their combinations forming a core-shell mixed structure at various CSR values, ranging from 0.1 to 0.9 with an increment of 0.1. This results in a total of 305 distinct and plausible aerosol components under consideration. This excludes combinations involving MD as the shell component and the homogenous internal mixing of these aerosol components, as their physical existence is rather unlikely in the atmosphere (Jacobson, 2000; Dey et al., 2008). The SU component is not explicitly considered, as the WS component accounts for anthropogenic sulfate. Different CSR values signify distinct mixing scenarios of core and shell components, each with varying mass fractions within a particle. For instance, a CSR of 0.1 indicates a thick coating, while a CSR of 0.9 suggests a thin coating.

Previous studies have assumed either the entire mass of the constituent aerosol components or a specific fraction of it to be involved in core-shell mixing (Chandra et al., 2004; Dey et al., 2008; Srivastava and Ramachandran, 2013). The latter assumption aligns more closely with observed mixing scenarios. Wherein, the entire mass of an aerosol component may not necessarily be in a core-shell mixed state with another. Instead, a fraction of it may be, while the rest can exist in an externally mixed state or be internally mixed with other aerosol components (Arimoto et al., 2006; Shamjad et al., 2016; Thamban et al., 2017). However, both assumptions necessitate prior knowledge of the component-wise M_a for computing the CSR value of core-shell mixed aerosols to determine their optical properties. In contrast, this study proposes allowing the variations of CSR values of core-shell mixed aerosols in the model. This offers a more flexible approach than relying on measured M_a to assess the probable aerosol mixing state. Subsequently, the mass fraction of the core and shell components participating in the mixing can be calculated from the CSR value of the probable core-shell mixed components using Eq. (1).

The aerosol mixing state in this study is described based on the distribution of the mass of different aerosol components within the aerosol mixture. If each particle in the mixture is composed of a single aerosol component, the mixture is considered 100% externally mixed. Conversely, if all the particles are composed of two aerosol components as a core-shell structure, it is denoted as 100% core-shell mixed. The total mass of the particles composed of a single aerosol component contributes to the externally mixed aerosol mass fraction, while the total mass of particles with a core-shell structure contributes to the core-shell mixed mass fraction. The mass fraction of an aerosol component in a core-shell mixed component is determined by calculating the ratio of its mass in that core-shell mixed component to the total mass of that component in the aerosol mixture. The masses of core and shell components in a core-shell mixed component are computed using Eq. (1). The combined mass of an aerosol component in various core-shell mixed particles and in an externally mixed state contributes to the total mass of that aerosol component in the mixture. The combined mass concentrations of SSam and SScm together are referred to as SS mass concentration (M_{SS}), while MDnm, MDam, and MDcm collectively constitute the MD mass concentration (M_{MD}). Here onwards, IS, WS, and BC mass concentrations are denoted as M_{IS}, $M_{WS,}$ and $M_{BC,}$ respectively. The scalability of AeroMix in terms of the number of components that can be defined in a given mixture enabled this study to assess the possible existence of different types of core-shell mixed particles in the atmosphere. Since AeroMix models optical properties at specified RH levels, the nearest RH value to the

seasonal average of the daytime mixed layer RH for Kanpur and the regional average for BoB is chosen, respectively.

3.2.3. Aerosol vertical profile

The vertical distribution of aerosols in the mixed layer is modeled by fitting a cubic polynomial (Eq. (6)) to the measured β_{ext} at 532 nm profiles. The choice to explore an alternative approach emerged because the exponential function (Eq. (5)) may not consistently capture the actual vertical variation of aerosols, particularly when there are co-existing elevated aerosol layers. This inconsistency results in an inaccurate representation of the measured β_{ext} profiles. In the cases examined in this study, the exponential function yielded a suboptimal fit, as indicated by R^2 values ranging from -0.24 to 0.7 and RMSE varying between 0.03 and 0.14. Conversely, the cubic polynomial provided the best fit, with R^2 and RMSE values ranging from 0.91 to 0.99 and 0.004 to 0.036, respectively. The aerosol chemical composition and vertical profiles in the free troposphere and stratosphere are modeled following Hess et al. (1998). The size distributions and optical properties of all aerosol components are assumed to be uniform throughout the atmospheric column.

Assessing the impact of these assumptions about the aerosol vertical profile is challenging due to the limitation in determining the extent of changes in aerosol properties with altitude. Even if such variations are known, like other inversion algorithms (Lewandowski et al., 2010; Sinha et al., 2013), there is a limitation associated with the Mie inversion technique in estimating the effect of the changes on the inversion results, although it has been widely utilized as described above. Alternatively, sensitivity estimates on AOD of the parameters describing vertical profiles are also complicated owing to the interdependence of multiple factors influencing AOD, such as vertical profile and layer thickness of aerosols. Suppose the covariation of the aerosol vertical profile with changes in mixed layer thickness is disregarded by assuming a constant aerosol vertical profile while varying the MLH. In that case, the changes in AOD ($\Delta AOD/\Delta MLH \approx \partial AOD/\partial h$) are minimal (<0.0005) for a unit meter shift in MLH across the different vertical profiles considered (Fig. S3). A detailed description of this sensitivity analysis is given in SI. However, the $\Delta AOD/\Delta MLH$ is not uniform throughout the vertical column. Instead, it follows the given vertical distribution of aerosols within the layer. This suggests that alterations in MLH have a more pronounced effect on AOD at altitudes characterized by higher aerosol concentrations than those with lower aerosol concentrations. Given the highly heterogeneous spatial and temporal nature of aerosol vertical distribution in the real atmosphere (Kumar et al., 2023), attempting a generalized quantification of the sensitivity of vertical profile assumptions on AOD lacks meaningful interpretation.

3.3. Assessment of probable aerosol mixing state

The probable existence of the aerosol components in the atmosphere, which refers to the aerosol mixing state is assessed by iteratively varying the number concentrations in the mixture in AeroMix until the root mean squared error (RMSE) between the measured and modeled AOD and SSA spectra are minimized. Only those spectra with RMSE minimum ≤ 0.03 are considered as the best fit (Fig. 1). The RMSE threshold of 0.03 is chosen to ensure that the RMSE remains within the lowest uncertainty (15%) in the Aerosol Robotic Network (AERONET) AOD and SSA retrievals (Srivastava and Ramachandran, 2013). Since AeroMix models optical properties at specific

wavelengths, modeled AOD values are interpolated to the measurement wavelengths for calculating the RMSE using a second-order polynomial equation (Eq. (8)) (Eck et al., 1999), which provides greater precision compared to the Ångström exponent power law.

$$ln\,AOD(\lambda) = a_2(ln\,\lambda)^2 + a_1\,ln\,\lambda + a_0 \qquad (3),$$

where λ is the wavelength at which AOD is calculated, and a_0, a_1, and a_2 are coefficients. However, for SSA, wavelengths closer to the measurement wavelengths are chosen in AeroMix since no equivalent relationship exists for SSA interpolation.

The aerosol mixtures with modeled spectral AODs and SSAs matched well with the measured ones (RMSE≤ 0.03) are taken as probable aerosol mixing states for a given location and season under consideration. It is important to note that the aerosol mixing state modeled by the Mie inversion technique is not unique but a probable scenario. Solving a system of equations with number of unknowns greater than the constraints poses an undetermined system having multiple solutions (Sumlin et al., 2018). Hence, a physically feasible solution is selected from the AeroMix-modeled probable aerosol mixing states by further constraining with the measured component-wise M_a with the modeled M_a agreed to within ±1σ. Measured M_a of organic carbon (OC), elemental carbon (EC), water-soluble organic carbon (WSOC), and water-soluble ionic species (WSIS) are grouped into the M_{IS}, M_{WS}, M_{BC}, $M_{SS,}$ and M_{MD} using appropriate fixed scaling factors for each component prescribed in the literature (see SI for detailed description). The asymmetry parameter is not considered to constrain the mixing states; however, a brief comparison between modeled and measured asymmetry parameter values is provided in the next section.
"

6. Little mention of future work/applications. Maybe mention potential model development projects and associated improvement to probable mixing state predictions.

   Reply: The lines #486-490 (Page #25) are revised as;

   "The prospective advancement linked to AeroMix involves the development of an optimization/machine learning algorithm utilizing AeroMix as the aerosol optical model. Such an algorithm will enable faster and more deterministic estimation of aerosol mixing states at fine temporal and spatial resolutions."

Minor comments

Line 43: Healy et al. 2014 and Ye et al. 2018 describe in situ measurements of mixing state between external and internal.

Reply: The single-particle mass spectrometry observations presented in these studies will help present the case in our manuscript. Suggested references are incorporated to strengthen the discussion on real atmospheric aerosol mixing states. The lines #47-50 (Page #2) are revised as;

"Despite the experimental evidence that the aerosol mixing state lies between a purely externally mixed state and a purely internally mixed state (Healy et al., 2014; Li et al., 2016; Ye et al., 2018; Riemer et al., 2019), the standard FORTRAN-based OPAC model considers the external mixing of aerosols alone and cannot treat complex aerosol internal mixing states."

Line 58: Unclear to reader why "batch mode" would have limited functionalities. Either clarify or reword.

Reply: We removed this discussion about AEROgui to avoid ambiguity (Page #2, Line #63).

Line 97-98: Unclear why density of BC is mentioned here.

Reply: The specific densities for all components are sourced from the Global Aerosol Data Set and OPAC database. However, the observational studies on black carbon suggest using a specific density value of 1.8 g cm^{-3}, differing from the 1.0 g cm^{-3} value provided in OPAC. The sentence is revised as follows (Page #5, Line#118)**:**

"The density of BC is set at 1.8 g cm^{-3} based on observations, which differs from the value of 1.0 g cm^{-3} given in OPAC (Bond et al., 2013; Kondo, 2015)."

Line 137 – 139: This sentence is confusing, specifically "and particles composed of multiple chemical species (internally mixed) as an external mixture."

Reply: The sentence (Page#5, line#94) is revised as follows for brevity.
"Optical properties of the complex aerosol mixing states are modeled by accounting for any number of both externally mixed particles (composed of single chemical species) and internally mixed particles (composed of multiple chemical species as core and shell), with no presumed chemical or physical interaction among the particles within the mixture (see Fig. 1)."

Equation (7): I believe index of summation should be layer, not n.

Reply: The equation is corrected as (Page #9, line# 191),
"

$$Total\ AOD = \sum_{n=1}^{6} \beta_{ext_n} \int_{h_{min_n}}^{h_{max_n}} N_n(h)dh$$

where h_{min} and h_{max} are the layer bottom and layer top height for each layer n."

Line 163: Consider adding one sentence on the Mie inversion technique.

Reply: The sentence is revised as follows (Page #10, Line #198):

"The probable aerosol mixing states are modeled with AeroMix using the Mie inversion technique by iteratively comparing the multispectral measurements of aerosol optical properties with modeled ones for different mixing scenarios until they converge within the observational error (Fig. 1) (Chandra et al., 2004; Dey et al., 2008; Kaskaoutis et al., 2011; Ramachandran and Srivastava, 2016; Srivastava et al., 2016, Srivastava et al., 2018)"

Figure 2: Consider adding average wind directions for winter, pre-monsoon and post-monsoon. This would aid in the comparison of modeled mixing states discussion (Sections 4.3 and 4.4). Label IGP region.

Reply: Average wind directions for different seasons are added to Figure 2, along with labeling the IGP region as shown below (Page #14).
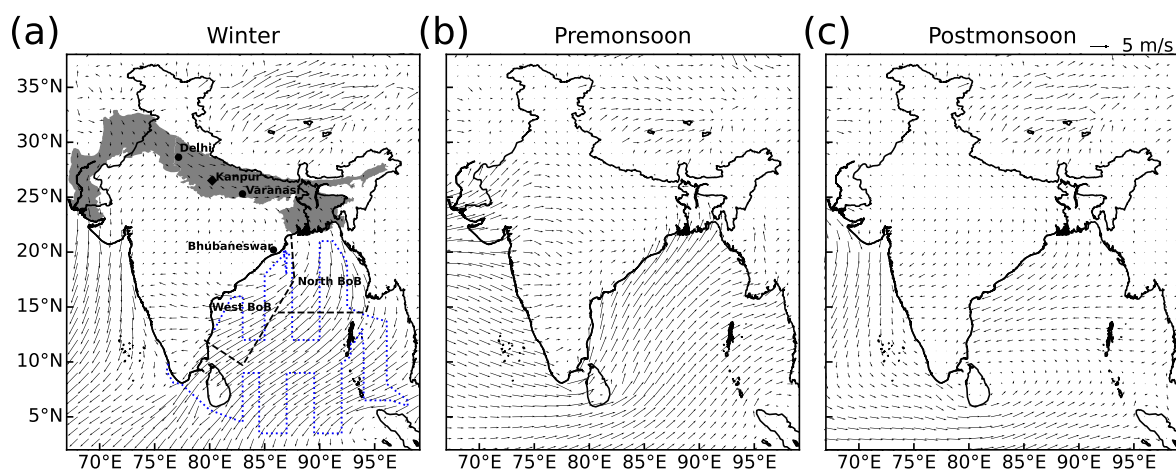
Figure 2: a) Location of Kanpur (diamond) and the W-ICARB cruise track (dotted lines). Measurements of AOD, chemical composition, and relative humidity over the West-BoB and North-BoB (demarcated with dashed lines) were utilized in this study. Additionally, the locations of Delhi, Varanasi, and Bhubaneswar (circles) are indicated, where mixing state measurements were obtained for comparison with the modeled mixing states. The shaded area marks the Indo-Gangetic Plains. Seasonal average surface winds over the region from ERA5 reanalysis are shown for a) winter, b) premonsoon and c) postmonsoon by vectors.

Line 243: Add reasoning for RMSE threshold after sentence: "Only those spectra with RMSE minimum 0.03 are considered as the best fit (Fig. 1). [Add here]." The last sentence of this paragraph "The RMSE threshold of 0.03 is chosen to ensure …" should be moved to this location.

Reply: Revised as suggested (Page #17, Line #311):

"Only those spectra with RMSE minimum ≤ 0.03 are considered as the best fit (Fig. 1). The RMSE threshold of 0.03 is chosen to ensure that the RMSE remains within the lowest uncertainty (15%) in the Aerosol Robotic Network (AERONET) AOD and SSA retrievals (Srivastava and Ramachandran, 2013)."

Figure 3 and 4: Unnecessary to include colors for externally mixed and core-shell mixed in caption.

Reply: Revised as suggested;

Page #20
"Figure 3: Measured and AeroMix modeled aerosol parameters over Kanpur during the winter, premonsoon, and postmonsoon seasons of 2007-2009. a) AeroMix modeled season-wise spectral AOD compared with AERONET measured AOD. Vertical bars represent the standard deviation of the mean values. Root mean square error of the fit is given in parenthesis, b) Same as (a) but for SSA, c) Component-wise aerosol mass concentration in externally mixed and core-shell mixed state compared with measured aerosol mass concentration. Vertical bars represent standard deviation of measurements, d) Modeled percentage mass fraction of aerosol components to the total aerosol mass (inner pie) and percentage mass fraction of externally mixed and core-shell mixed aerosols to the total aerosol mass (outer pie)."

Page #22
"Figure 4: Measured and AeroMix modeled aerosol parameters over W-BoB and N-BoB during winter season (December 2008-January 2009). a) AeroMix modeled season-wise spectral AOD compared with measured AOD. Vertical bars represent the standard deviation of the mean values. Root mean square error of the fit is given in parenthesis, b) Component-wise aerosol mass concentration in externally mixed and core-shell mixed state compared with measured aerosol mass concentration. Vertical bars represent standard deviation of measurements, c) Modeled percentage mass fraction of aerosol components to the total aerosol mass (inner pie) and percentage mass fraction of externally mixed and core-shell mixed aerosols to the total aerosol mass (outer pie)."

Technical corrections

Line 11: Add comma after "aerosol chemical compositions,"

Reply: Corrected as suggested (Page #1, Line #11):

"Assessing aerosol mixing states, which mainly depend on aerosol chemical compositions, is indispensable for estimating aerosol direct and indirect effects."

Line 13: Remove "the" so the sentence reads "While limitations in the measurements of aerosol …"

Reply: The sentence is modified as per the next comment.

Line 13-15: Sentence "While the limitations in the measurements …" is a run on. Consider breaking into two sentences.

Reply: Following your suggestion, we corrected the sentence as (Page #1, Line #12):

"The limitations in the direct measurements of aerosol chemical composition and mixing states necessitate modeling approaches to infer the aerosol mixing states. The Optical Properties of Aerosols and Clouds (OPAC) model has been extensively utilized to construct optically equivalent aerosol chemical compositions from measured aerosol optical properties using Mie inversion."

Line 18: Move position of "3)" – "components, and 3) define aerosol composition"

Reply: Corrected as suggested (Page #1, Line #19):

"2) simulate optical properties of aerosol mixtures constituted by any number of aerosol components, and 3) define aerosol composition and relative humidity in up to six vertical layers."

Line 98: Add comma "The optical properties of each component, except for the MD components, are calculated"

Reply: Corrected as suggested (Page 5, Lines #119-121):

"The optical properties of each component, except for MDnm, MDam, and MDcm components, are calculated using the Mie theory (Mie, 1908)."

Line 209: Run-on sentence, rewrite as "…CSR values of core-shell mixed aerosols in the model. This offers a more flexible approach compared to relying on measured…"

Reply: Corrected as suggested (Page #15, Line #261):

"In contrast, this study proposes allowing the variations of CSR values of core-shell mixed aerosols in the model. This offers a more flexible approach than relying on measured M_a to assess the probable aerosol mixing state."

Line 297: Change to "… mixed states varied from 30% to 59% in premonsoon and winter, **respectively."**

Reply: Changing to "mixed states varied from 30% to 59% in premonsoon and winter, respectively" may lead to confusion regarding whether these values represent intra-seasonal or inter-seasonal variation. To clarify, we have revised the line #374 (Page #21):

"The percentage mass fractions of the total M_a in core-shell mixed states increased from 30% in premonsoon to 59% in winter (Fig. 3d)."

This manuscript is generally well-composed.

Reply: We appreciate and thank the reviewer for his/her constructive comment and recommendation. We have incorporated the necessary corrections in the revised manuscript as described below.

Dividing the content between lines 80 to 120 into more succinct paragraphs could significantly improve readability.

Reply: Following your suggestion, we have divided section 2 into two subsections and added a table to explain pre-defined components to improve readability. Section 2 is restructured and revised as follows (Pages #3-10, Lines #80-195).
"

2. Model overview

AeroMix is an open-source Python package developed to model the optical properties of aerosol mixtures, including AOD, SSA, asymmetry parameter, extinction coefficient (β_{ext}), scattering coefficient (β_{sca}), and absorption coefficient (β_{abs}) at sixty-one wavelengths ranging from 0.25 to 40 µm and eight relative humidity (RH) values, following Hess et al. (1998). The workflow of AeroMix for modeling the aerosol properties and assessing the probable mixing states is illustrated in Fig. 1. A methodology for modeling the probable aerosol mixing state using AeroMix is detailed in the subsequent section.

2.1. Mixing of aerosol components

Aerosol mixtures in AeroMix can be defined in terms of the number or mass concentration of the constituent aerosol components in external and/or internal (core-shell) mixed states, along with their vertical distribution and the vertical profile of RH. Optical properties of the complex aerosol mixing states are modeled by accounting for any number of both externally mixed particles (composed of single chemical species) and internally mixed particles (composed of multiple chemical species as core and shell), with no presumed chemical or physical interaction among the particles within the mixture (see Fig. 1).

2.1.1. Externally mixed aerosol components

Nine predefined externally mixed aerosol components in AeroMix include water-insoluble (IS), water-soluble (WS), black carbon (BC), accumulation and coarse modes of sea-salt (SSam and SScm), nucleation, accumulation and coarse modes of mineral dust (MDnm, MDam, and MDcm) and stratospheric sulfate (SU). These components are represented in terms of their lognormal size distribution parameters (geometric standard deviation (σ), mode radius (r_m) and the upper and lower limits of radius, r_{min} and r_{max}), specific density (ρ), spectral refractive indices (m) and optical properties averaged for one particle ($\beta_{ext}(\lambda)$, $\beta_{sca}(\lambda)$, $\beta_{abs}(\lambda)$, SSA (λ)

and g (λ)) at sixty-one wavelengths from 0.25 to 40 µm and eight RH values, adopted from the Global Aerosol Data Set and OPAC database (Koepke et al., 1997; Hess et al., 1998; Koepke et al., 2015). A brief overview of the parameters used to describe the predefined aerosol components at dry state (0% RH) is given in Table 1. Detailed descriptions of the aerosol components, along with their size distribution parameters and spectral refractive indices, can be found elsewhere (Koepke et al., 1997; Hess et al., 1998; Koepke et al., 2015). The density of BC is set at 1.8 g cm^{-3} based on observations, which differs from the value of 1.0 g cm^{-3} given in OPAC (Bond et al., 2013; Kondo, 2015). The optical properties of each component, except for MDnm, MDam, and MDcm components, are calculated using the Mie theory (Mie, 1908). This calculation assumes that the particles are spherical in shape and follow a lognormal size distribution. The calculated optical properties are normalized to one particle cm^{-3} and stored, which can then be scaled to any given number concentration. MDnm, MDam, and MDcm components are modeled using the T-Matrix Method (TMM) (Waterman, 1971; Mishchenko et al., 1999) to account for their non-sphericity (Koepke et al., 2015). In addition to the nine predefined aerosol components, AeroMix offers the flexibility to model any number of user-defined components. A new externally mixed aerosol component can be defined in AeroMix by its size distribution parameters, specific density, and spectral refractive indices described above.

Table 2: Size distribution parameters, specific densities, and refractive indices of predefined aerosol components at dry state (0% RH).

Aerosol component	Constituting species	Mode radius (µm)	Geometric standard deviation	specific density (g cm^{-3})	Refractive index at 0.5 µm
Insoluble (IS)	Soil dust, fly ash, and non-hygroscopic organic matter.	0.471	2.51	2.0	$1.53 + 8 \times 10^{-3}$i
Water-soluble (WS)	$SO_4^{2-}, NO_3^-, NH_4^+$ and hygroscopic fraction of organic matter.	0.0212	2.24	1.8	$1.53 + 5 \times 10^{-3}$i
Black carbon (BC)	Black carbon aerosols	0.0118	2	1.8	$1.75 + 4.5 \times 10^{-1}$i
Sea-salt accumulation mode (SSam)	Sea salt aerosols	0.209	2.03	2.2	$1.5 + 1.55 \times 10^{-8}$i
Sea-salt coarse mode (SSam)		1.75	2.03		
Mineral dust nucleation mode (MDnm)	Desert dust	0.007	1.95	2.6	$1.53 + 7.8 \times 10^{-3}$i
Mineral dust accumulation mode		0.39	2		

(MDam)					
Mineral dust coarse mode (MDcm)		1.9	2.15		
Stratospheric sulfate (SU)	Sulfate aerosols from volcanic eruption.	0.0695	2.03	1.7	$1.431 + 1 \times 10^{-8}$i

The OPAC aerosol database is comprehensive, reliable, based on extensive observations, and widely employed in radiative transfer modeling, global climate modeling, and mixing state studies (Shettle et al., 1979; Deepak and Gerber, 1983; Koepke et al., 1997; Srivastava et al., 2016). Studies examining the sensitivity of refractive indices report negligible influences on modeled β_{ext} (Ramachandran and Jayaraman, 2002; Srivastava et al., 2016). Further, Srivastava et al. (2016) investigated the sensitivity of BC mode radius on SSA and β_{ext} for BC and sulfate in different mixing states, revealing differences of only up to 1.3%. Hence, the AeroMix modeled optical properties using the OPAC database are anticipated to be minimally affected by uncertainties in refractive indices and size distribution parameters. Along with the default database, AeroMix allows users to employ various datasets that characterize aerosols using the parameters described above. This flexibility not only enables users to choose datasets based on their preferences but also enhances AeroMix capability by incorporating more comprehensive datasets that consider the complex characteristics of aerosol particles, including morphology.

2.1.2. Internally mixed aerosol components

 Core-shell mixed aerosol components can be defined in AeroMix by specifying the core and shell components with their core-to-shell radius ratio (CSR) or mass fractions of the species in a core-shell mixed particle. Optical properties of the core-shell mixed aerosol components are modeled by using PyMieScatt (Sumlin et al., 2018), a coated-sphere Python Mie calculation program based on the BHCOAT program (Bohren and Huffman, 1998). PyMieScatt takes the spectral refractive indices of the core and shell components, and the radius of the core (r_c) and shell (r_s) as input parameters to model the optical properties of the core-shell mixed components.
The r_s for each particle is equivalent to the radius of the core-shell mixed particle and is assumed to follow the size distribution of the shell component (Srivastava et al., 2016), which is also supported by observations (Arimoto et al., 2006). The r_c of each particle is calculated according to the CSR, expressed as the ratio of the r_c to the r_s, and is given by,

$$CSR = \frac{r_c}{r_s} = \left(1 + \frac{M_s \rho_c}{M_c \rho_s}\right)^{(-1/3)}, \tag{4}$$

M_c and M_s are the mass contributions of core and shell components to the mixing, and ρ_c and ρ_s are the specific mass densities of core and shell components, respectively (Srivastava et al., 2016; Chandra et al., 2004). CSR can be specified in AeroMix either directly or in terms of the mass contribution of the core and shell components. The mass of the core-shell mixed components is calculated from their size distribution parameters and effective mass density (ρ_{eff}). The ρ_{eff} of the core-shell mixed particle can be defined as,

$$\rho_{eff} = \frac{M_c + M_s}{V}, \tag{5}$$

where V is the volume of the core-shell mixed particle. Since M_c, M_s, and V vary along the particle size distribution as a function of r_c and r_s, ρ_{eff} needs to be defined in terms of parameters that remain fixed across the size distribution for modeling simplicity. For this, M_c and M_s can be written as,

$$M_c = \rho_c \frac{4}{3}\pi r_c^3 \text{ and } M_s = \rho_s \frac{4}{3}\pi(r_s^3 - r_c^3). \tag{6}$$

Since, $CSR = \frac{r_c}{r_s}$,

$$\rho_{eff} = \rho_c CSR^3 + \rho_s(1 - CSR^3). \tag{7}$$

Equation (4) contains only the terms of the specific density (ρ) of core and shell components and CSR value, which remain the same across the size distribution.

2.2. Vertical profiles of aerosols and relative humidity

For total column AOD calculation, up to six vertically arranged layers can be defined to specify the vertical distribution of aerosols. Unlike OPAC, in AeroMix, aerosol concentrations at the layer base, aerosol profile type, and layer mean RH can be defined separately for mixed layer, free troposphere, stratosphere, and elevated aerosol layers. In contrast, OPAC uses constant background extinction coefficient values and RH for the free troposphere and stratosphere. The vertical profile of aerosol concentration in each layer can be modeled as homogenous or as an exponential function given by,

$$N(h) = N(0)exp\left(-h/z\right), \tag{8}$$

where $N(0)$ is the number concentration of aerosol at the layer bottom, h is the height from the layer bottom, and z is the scale height representing the change in aerosol concentration with height (Hess et al., 1998). Standard exponential profiles for different aerosol types provided by Hess et al. (1998) can be utilized for locations lacking aerosol vertical profile measurements. Alternatively, it can be modeled using a cubic function (Eq. (6)) when aerosol vertical profile measurements are available.

$$N(h) = N(0)(ah^3 + bh^2 + ch + d), \tag{9}$$

where a, b, c, and d are the coefficients when $N(0) = 1$ (Russo et al., 2006). The default values of aerosol concentration, RH, and profile type for the free troposphere, stratosphere, and elevated mineral dust layer are adopted from Hess et al. (1998). The total column AOD is calculated by,

$$Total\ AOD = \sum_{n=1}^{6} \beta_{ext_n} \int_{h_{min_n}}^{h_{max_n}} N_n(h)dh \tag{10}$$

where h_{min} and h_{max} are the layer bottom and layer top height for each layer n.

The AeroMix package and detailed documentation are available online at www.github.com/sampr7/AeroMix (P Raj and Sinha, 2024a).

Reviewer: # 3

Overall the paper is written and presented very well, though I agree with the other referees about rearranging section 3 to make a smoother read.
Verdict: Accept with minor revisions (detailed below)

Reply: We appreciate and thank the reviewer's insightful and detailed comments and recommendation. All comments have been taken into account, as described below.
We have also restructured sections 2 and 3 following the first and second reviewer's comments.

General Comments

1. In the introduction (e.g. line 53), the limit on number of aerosol components that are available in OPAC is presented as a key limitation on its ability to infer mixing state. However, on line 103, the authors explain how AeroMix relies on the OPAC aerosol database for its measurements. My understanding is that AeroMix is therefore limited to the number of components available in the OPAC aerosol database. Therefore, whilst both OPAC and AeroMix rely on the OPAC aerosol database, are they not identically limited to the number of aerosol components? (By the way, I note there is an argument that users could append aerosol components to the OPAC aerosol database, and therefore extend the number of aerosol components present in AeroMix, but is this not equally true for the OPAC model? If not, then please explain.)

Reply: While both OPAC and AeroMix use the OPAC aerosol database, the limitation of OPAC is not due to the number of components available in the database (which are nine). It is due to the maximum number of components permissible in a mixture is seven for calculating the optical properties. This is specified in the OPAC input file as depicted below.

> *# if you did select 0 (define new mixture), in the next 5 lines the*
> *# component number and the number density in [particles/cm**3] has to be*
> *# given, divided by commas. The component numbers are the following:*
> *#*
> ***# There are not more than 7 components allowed to compose one aerosol***
> ***# or cloud type.***
> *#*
> *# (1) insoluble   (6) mineral (nuclei mode, nonspherical)*
> *# (2) water-soluble   (7) mineral (accumulation mode, nonspherical)*
> *# (3) soot   (8) mineral (coarse mode, nonspherical)*
> *# (4) sea-salt (accumulation mode)*
> *# (5) sea-salt (coarse mode) (10) sulfate*

In contrast, AeroMix offers more flexibility, which can account for any number of aerosol components to constitute a mixture. It does utilize all the nine predefined components available in the OPAC database. In

addition, it also allows user-defined aerosols in the mixture as explained in lines #124-127. In this study, along with the predefined components, their core-shell mixed combinations at various mass mixing ratios are also considered, totaling 305 components as explained in line #247.

Adding new aerosol components to OPAC would require compromising the predefined components due to the program's limitation to account for more than seven components in a mixture. With the capability of AeroMix to model any number of aerosol components in a mixture, this study assessed the probable coexistence of aerosol components in externally mixed states and different core-shell mixed states at various mass-mixing scenarios, considering all possibilities simultaneously, which is why we believe it offers a more comprehensive approach to assessing the aerosol mixing state as explained in line #387.

2. It is clear from Fig. 1 that AeroMix, as a stand-alone model predicts the optical properties of aerosol populations, and I can see from line 73 and line 98 that (as in OPAC) Mie theory is used to do this, and this is represented by the 'AeroMix' item in Figure 1. However, I am confused by the Mie inversion part of AeroMix: in line 163 several references are given for the 'Mie inversion' technique to find the aerosol mixing state, however none of these references use the phrase 'Mie inversion' for their techniques. Is this phrase newly coined in this paper? If so, it should be properly justified, including an explanation of why 'inversion' is the correct word, rather than iteration. I say this because it appears from Fig 1 and the description in line 241-260 that an iterative approach is used to find the mixing state that gives best fit to observations. Therefore, I question whether this is an inversion approach, or an iterative approach. Would 'Mie iteration' be a better phrase?

Reply: We acknowledge that the term 'Mie inversion' is not used in any of the cited references. However, related phrases such as 'inverting Mie model' or 'inverse Mie problem' are frequently used when estimating aerosol properties like refractive indices from optical properties. For example, Sumlin et al. (2018) discuss solving the 'inverse Mie problem' for a complex refractive index given inputs of scattering, absorption, and size distribution parameters. Similarly, Pedrós et al. (2014) refer to 'inverting the Mie model' to infer aerosol properties from measured optical properties.

The forward Mie calculation process involves determining scattering and absorption parameters at specific wavelengths by inputting the radius and complex refractive index of the particle. Consequently, estimating particle properties, in this case, the aerosol component characterized by its spectral refractive indices and size distribution parameters, from measured optical properties, presents an inverse Mie problem. The solution to this problem is obtained by iteratively finding a combination of aerosol components (an aerosol mixture) that yields aerosol optical depth and single scattering albedo spectra that best match the measured ones, with a minimum root mean square error (RMSE) between the modeled and measured spectra (as explained in line #309).

Given the context above, we believe the term 'Mie inversion' is more appropriate than 'Mie iteration', as it accurately reflects the process of solving the inverse problem, even though it involves iterative steps.

3. Line 241 indicates that the iteration in AeroMix finds the probable existence of components, but Fig 1 and other part of the main text (e.g. line 253) suggest the iteration finds the probable mixing state. What does the iteration solve? Is it both the components present and their mixing state? If so, please make clearer.

Reply: The iteration specifically solves for the number concentration of aerosol components, with non-zero values indicating the probable existence of these components which refers to the aerosol mixing state. Line #309 (Page #17) is revised as follows for clarity:

"The probable existence of the aerosol components in the atmosphere, which refers to the aerosol mixing state is assessed by iteratively varying the number concentrations in the mixture in AeroMix until the root mean squared error (RMSE) between the measured and modeled AOD and SSA spectra are minimized."

4. The authors acknowledge that the iterative technique used to estimate probable mixing states is not unique (line 254). I would like to see more discussion, or reference (where this issue has been detailed before), around the range of mixing states that can be inferred from the iteration technique for a given set of inputs, i.e., a discussion around the probability that a given inferred mixing state is accurate. If I understand that AeroMix returns just one probable mixing state for a given set of inputs, then this seems to me to be a fundamental weakness, and future work should prioritise quantifying the uncertainty around the returned mixing state, and/or returning multiple mixing states so that users can quantify the range of probable solutions. I see that this issue is dealt with in lines 404-407, which explains that other algorithms could imbed AeroMix and therefore quantify the probable accuracy of returned mixing states. I also see that in sections 4.4 and 5, that the authors express the limitations of AeroMix, stating that only results useful for qualitative interpretation are returned. This is great, because it's key that the authors describe the model's limitations. However, I think this limitation should be mentioned in the model overview, so that readers are quickly aware of it. Furthermore, it would be useful to have some more description around what the 'inherent constraints' mentioned in line 401 are – this would greatly help authors of future minimization and machine learning algorithms to correctly utilise AeroMix.

Reply: The above reviewer comment has been segmented into four distinct sections for a more structured response:

    a) The authors acknowledge that the iterative technique used to estimate probable mixing states is not unique (line 254). I would like to see more discussion, or reference (where this issue has been detailed before), around the range of mixing states that can be inferred from the iteration technique for a given set of inputs, i.e., a discussion around the probability that a given inferred mixing state is accurate.

    We have mentioned in line #328 that the aerosol mixing state modeled by the Mie inversion technique is not unique, but a probable one. When solving a system of linear equations where the number of unknowns (number concentration of aerosol components) is greater than the number of constraints (spectral AODs and SSAs), multiple solutions are possible. This is because there are insufficient constraints to uniquely determine all the unknowns. While many possible solutions exist mathematically, not all are physically feasible for aerosols. To select a physically feasible solution for the location under consideration, we further constrained the modeled mixing states with concurrent and collocated measurements of component-wise aerosol mass concentration (Page #17, Line #332). The solutions in which the total aerosol mass concentration of each component (externally and core-shell mixed mass combined as explained in lines #267-275) within the bounds of $\pm 1\sigma$ of the measured component-wise aerosol mass concentration is considered acceptable.

We have revised line #328 (Page #17) to clarify this point as follows.

"It is important to note that the aerosol mixing state modeled by the Mie inversion technique is not unique but a probable scenario. Solving a system of equations with number of unknowns greater than the constraints poses an undetermined system having multiple solutions (Sumlin et al., 2018). Hence, a physically feasible solution is selected from the AeroMix-modeled probable aerosol mixing states by further constraining with the measured component-wise M_a with the modeled M_a agreed to within $\pm 1\sigma$."

b) If I understand that AeroMix returns just one probable mixing state for a given set of inputs, then this seems to me to be a fundamental weakness, and future work should prioritise quantifying the uncertainty around the returned mixing state, and/or returning multiple mixing states so that users can quantify the range of probable solutions. I see that this issue is dealt with in lines 404-407, which explains that other algorithms could imbed AeroMix and therefore quantify the probable accuracy of returned mixing states.

As explained above, AeroMix provides not just one solution for a given set of inputs, but different probable ones depending on the combinations examined. The key limitation of this technique is that it does not guarantee a unique solution but a probable one. To assess the probability of a particular solution being true or to quantify the range of uncertainty of the solution, all possible solutions need to be modeled. This is not practical considering the number of combinations to be examined and the required computational time. For example, if we check 1000 possible values for all 305 components, the total iterations required will be 1000^{305}. As the reviewer suggested for future work, the development of minimization and machine learning algorithms is already underway to ensure a quantitative and deterministic estimation of aerosol mixing states using AeroMix as discussed in lines #486-490 (Page #25).

c) I also see that in sections 4.4 and 5, that the authors express the limitations of AeroMix, stating that only results useful for qualitative interpretation are returned. This is great, because it's key that the authors describe the model's limitations. However, I think this limitation should be mentioned in the model overview, so that readers are quickly aware of it.

The limitation of the AeroMix in modeling aerosol mixing states using the Mie inversion technique is that the modeled mixing states are not unique, but probable scenarios. This inherently limits the analysis of mixing states using AeroMix to a qualitative examination. Lines #83-86 (Page #3) in the model overview section are revised as follows to indicate that the modeled mixing states are probable ones.

"The workflow of AeroMix for modeling the aerosol properties and assessing the probable mixing states is illustrated in Fig. 1. A methodology for modeling the probable aerosol mixing state using AeroMix is detailed in the subsequent section."

d) Furthermore, it would be useful to have some more description around what the 'inherent constraints' mentioned in line 401 are – this would greatly help authors of future minimization and machine learning algorithms to correctly utilise AeroMix.

The inherent limitations of the Mie inversion technique are detailed in response to the first part of this comment (a) as well as in section 3.3 in the revised manuscript. Lines #481-483 in Section 5 are revised to reflect this.

"However, this study is limited to a qualitative examination of aerosol mixing states due to the inherent constraints of the inverted Mie model approach as discussed in Sect. 3.3."

5. Please detail what happens along the 'No' route of Fig. 1 – the authors explain in line 241 that iterative changes are made, but how is the amount and direction of change estimated?

Reply: The direction of change is decided towards where the root mean square error between the modeled and measured AOD and SSA spectra are converged as mentioned in lines #309-311 (Page #17). Determination of the amount of change of component number concentration is under development and will be addressed in future work.

Minor Comments

Line 35 – please provide some example references of studies that have used OPAC to estimate probable mixing state.

Reply: The references cited in lines #49 and #163 have used OPAC to estimate the probable mixing state.

Line 57 – more detail is needed about why AEROgui is inferior to AeroMix, so that readers can distinguish between the two. For example, what limits in functionality does AEROgui have that AeroMix overcomes?

Reply: We removed this discussion about AEROgui to avoid ambiguity following the first reviewer's comment.

Line 137 – I don't understand the sentence starting on this line. Specifically, how can an internally mixed aerosol be treated as an external mixture? This sounds like the components comprising the internally mixed aerosol are separated into separate particles so that an external mixture is formed.

Reply: To clarify, for the Mie inversion technique, all the probable aerosol components need to be modeled in AeroMix beforehand to examine their existence in the mixture. Core-shell mixed aerosols are modeled as user-defined aerosol components, as explained in section 2.1.2 (Page #8) before they are constituted into a mixture. AeroMix treats this core-shell mixed aerosol in the same manner as an externally mixed aerosol. In other words,

for AeroMix, a core-shell mixed aerosol is another aerosol with characteristic spectral Mie coefficients, size distribution parameters, and specific density (ρ). However, these Mie coefficients are calculated using the coated-sphere Mie scattering theory and specific density as explained in line #158. AeroMix assumes no chemical or physical interaction among the particles within the mixture while calculating the optical properties.

Subsequently, different combinations of predefined externally mixed aerosols (composed of single chemical species) and internally (core-shell) mixed aerosols (composed of multiple chemical species) are used to constitute various aerosol mixtures in AeroMix to calculate their optical properties.

The sentence (Page #5, Lines #94-96) is revised as follows for brevity.

"Optical properties of the complex aerosol mixing states are modeled by accounting for any number of both externally mixed particles (composed of single chemical species) and internally mixed particles (composed of multiple chemical species as core and shell), with no presumed chemical or physical interaction among the particles within the mixture (see Fig. 1)."

References

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Sumlin, B. J., Heinson, W. R., and Chakrabarty, R. K.: Retrieving the aerosol complex refractive index using PyMieScatt: A Mie computational package with visualization capabilities, J. Quant. Spectrosc. Radiat. Transf., 205, 127–134, https://doi.org/10.1016/J.JQSRT.2017.10.012, 2018.