Code and Data Files Accompanying: Retrieval of the Sea Spray Aerosol Mode from Submicron Particle Size Distributions and Supermicron Scattering during LASIC

Authors: Dedrick, J.L.; Saliba, G.; Williams, A.S.; Russell, L.M.; Lubin, D.
Contact: Jeramy Dedrick. jdedrick@ucsd.edu. https://orcid.org/0000-0003-3569-0235. Scripps Institution of Oceanography, University of California San Diego, La Jolla, CA 92037.

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ABSTRACT:
This work reports on a new inverse Mie method to retrieve size-resolved sea spray concentration by combining submicron particle size distributions and sub-1 μm and sub-10 μm scattering difference from a 3-wavelength integrating nephelometer. The method was applied to clean marine observations during the Department of Energy Atmospheric Radiation Measurement Layered Atlantic Smoke Interactions with Clouds (LASIC) campaign on Ascension Island (Zuidema et al., 2016) and North Atlantic ship-based measurements during the first cruise of the NASA North Atlantic Aerosols and Marine Ecosystems Study (NAAMES) (Behrenfeld et al., 2019). In this document we detail the codes used to simulate sea spray scattering and retrieve sea spray modal fitting parameters as well as data applying these methods to LASIC and NAAMES.

SOFTWARE IMPLEMENTATION:
The codes necessary to execute the sea spray mode retrieval and simulate sea spray mode scattering are provided within this digital collection (https://doi.org/10.6075/J0GT5NCR) and can be found in the Github code repository (https://github.com/jdedrick95/get_sea_spray_mode). Retrieved sea spray mode parameters from LASIC and NAAMES are also provided. All codes were written to run on MATLAB version R2019b. To replicate the results found in this paper, LASIC data can be found at https://adc.arm.gov/discovery/ while NAAMES data are archived at https://library.ucsd.edu/dc/object/bb0856963d.

CODE AND DATA LISTING:
get_sea_spray_mode.m
Written by: Jeramy L. Dedrick, Scripps Institution of Oceanography, 13 May 2021
Last edited 19 April 2022
Code repository: https://github.com/jdedrick95/get_sea_spray_mode

This MATLAB function retrieves lognormal fitting parameters of the sea spray mode using submicron size distributions and supermicron scattering. The code requires the sea spray Mie scattering look-up table (**sea_spray_mie_table.mat**) to be in the same directory as the retrieval code (or accessible from a working directory).

Inputs	
Variable	**Description**
bsca_RGB	supermicron scattering coefficients (Mm^{-1}) row dimension: time column dimension: [450nm, 550nm, 700nm]
bsca_std	standard deviation of supermicron scattering coefficients (Mm^{-1}) during temporal average row dimension: time

	column dimension: [450nm, 550nm, 700nm]
bsca_inst_std	instrument scattering error/uncertainty (%), single value (e.g. 5% (Frie and Bahreini, 2021))
PNSD	submicron particle size distribution (cm^{-3} μm^{-1}) row dimension: concentration column dimension: time
PNSD_D	submicron particle diameters from size distribution (µm) row dimension: diameters
D_op	overlap region for which to constrain Mie solutions (this variable is a user specified selection of diameters from PNSD_D) row dimension: diameters
PNSD_std	standard deviation of particle size distribution during temporal average; resolved at each size bin (cm^{-3} μm^{-1}) row dimension: concentration column dimension: time
PNSD_N_std	Instrument concentration error/uncertainty (%), single value (e.g. 10% (Frie and Bahreini, 2021))
PNSD_D_std	Instrument sizing uncertainty (%), single value (e.g. 2.5%, DMT UHSAS sizing uncertainty)

Outputs An example output file is provided as **sea_spray_out_example.mat**	
Variable	**Description**
sea_spray_mode	sea spray mode fitting parameters row dimension: time column dimension: [number, mean diameter, geometric standard deviation]
sea_spray_mode_95	95% confidence interval ranges of the sea spray mode fitting parameters. This variable is a cell matrix. row dimension: [number, mean diameter, geometric standard deviation] columns dimension: [lower 95^{th}, upper 95^{th}] cell dimension: time
error_thresh	scattering error threshold (Mm^{-1}) row dimension: time
low_error_idx	indices of the look-up table that fall below the error threshold. This variable is a cell matrix. row dimension: Mie look-up table indices cell dimension: time
test_coeff	probable Mie solutions that are tested against the measured size distribution. This variable is a cell matrix. row dimension: probable Mie solutions cell dimension: time
RSS_fit	residual sum of squares of unique sea spray mode to measured size distribution row dimension: time
chi2_fit	chi-square error of unique sea spray mode to measured size distribution

	row dimension: time
D_mie	size distribution diameters (μm)
dlogDp_mie	log-base 10 difference of the diameters
fail_flag	flag value identifying reason for retrieval failure (0 = retrieval successful, 1 = scattering not available at all 3 wavelengths, 2 = no Mie scattering solutions below the error threshold, 3 = no Mie solutions that are within the joint probability 95th percentile that can be tested against the size distribution) row dimension: time
retrieval_duration	time to complete the retrieval (minutes) row dimension: time

sea_spray_mie_table.mat
This MATLAB data matrix file contains a look-up table of scattering coefficients (b_sca) at 450nm, 550nm, and 700nm light wavelengths derived from the Mie code (**POLYDISP_SEA_SPRAY_MIE_CODE.m**) with a dry sea salt refractive index of 1.56 + 0i. The column dimensions are scattering at 450nm, 550nm, and 700nm and the row dimensions are scattering values attributable to the combinations of sea spray mode fitting parameters (coeff), which have column dimensions of the number concentration, geometric mean diameter, and geometric standard deviation. The variable D is the diameter range over which the size distribution and scattering coefficients are integrated.

sea_spray_out_example.mat
This MATLAB data matrix file provides an example output of the **get_sea_spray_mode.m** code applied to 2-hr clean marine period data during LASIC. See the output section of **get_sea_spray_mode.m** description for details**.**

POLYDISP_SEA_SPRAY_MIE_CODE.m
Written by: Geroges Saliba, Scripps Institution of Oceanography, 21 November 2019
Last edited by Jeramy L. Dedrick, 16 January 2022

This code simulates the Mie scattering coefficients (b_sca) for sea spray size distributions defined by scattering wavelengths (lemda) and size distribution parameters (N, Sigma, mu; coeff). The function cites Mie scattering equations from (Bohren and Huffman, 1998) and sea salt refractive index from (Kent et al., 1983). The functions **Mie_abcd.m** and **Mie_abcd_coating.m** are required to be in the same directory as the retrieval code (or accessible from a working directory). Sea spray mode look-up tables can be compiled by saving the variables b_sca, coeff, and D.

Mie_abcd.m
Written by: Christian Mätzler, Institute of Applied Physics, University of Bern, June 2002
Edited by Georges Saliba, Scripps Institution of Oceanography, 21 January 2020
Last edited by Jeramy L. Dedrick, 16 January 2022

This function computes a matrix of Mie coefficients, a_n, b_n, c_n, d_n, of orders n=1 to nmax, complex refractive index (m=m'+im"), and size parameter x = k0*a, where k0= wave number in

the ambient medium, a=sphere radius. This function cites Mie equations from (Bohren and Huffman, 1998) and implements the Mie_abcd procedure of (Mätzler, 2002).

Mie_abcd_coating.m
Written by: Christian Mätzler, Institute of Applied Physics, University of Bern, June 2002
Edited by Georges Saliba, Scripps Institution of Oceanography, 21 January 2020
Last edited by Jeramy L. Dedrick, 16 January 2022

This function computes a matrix of Mie coating coefficients, a_n, b_n, c_n, d_n, of orders n=1 to nmax, complex refractive index (m=m'+im"), and size parameter x = k0*a, where k0= wave number in the ambient medium, a=sphere radius. This function cites Mie equations from (Bohren and Huffman, 1998) and implements the Mie_abcd_coating procedure of (Mätzler, 2002).

LASIC_sea_spray_UHSASNEPH.txt
This text file contains the sea spray mode fitting parameters retrieved from Ultra-High Sensitivity Aerosol Spectrometer (UHSAS) size distributions and nephelometer scattering coefficients during 2-hr clean marine periods of LASIC.

LASIC_sea_spray_UHSASONLY.txt
This text file contains the sea spray mode fitting parameters retrieved using only the UHSAS size distribution as detailed in (Saliba et al., 2019; Sanchez et al., 2021) for 2-hr clean marine periods of LASIC.

NAAMES_sea_spray_SEMSAPS.txt
This text file contains the sea spray mode fitting parameters retrieved through merger of the Scanning Electrical Mobility Sizer (SEMS) and Aerodynamic Particle Sizer (APS) as detailed in (Saliba et al., 2019) for 2-hr clean marine periods of NAAMES1.

NAAMES_sea_spray_SEMSNEPH.txt
This text file contains the sea spray mode fitting parameters retrieved from SEMS and nephelometer scattering coefficients during 2-hr clean marine periods of NAAMES1.

SUPPORT:
Users can seek support for these codes by emailing Jeramy Dedrick (jdedrick@ucsd.edu).

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