

DATASET CATALOG

Optical Modeling of Single Asian Dust and Marine Air Particles: A Comparison with Geometric Particle Shapes for Remote Sensing

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CONTENTS OF DATASET

The dataset consists of Microsoft Excel and Word files, text files, and bitmap image files. The Asian dust particles are labeled: CaMg 1D, CaMg 2N, CaMg 3D, CaMg 4N1, Ca-rich 1D, Ca-rich 2N, Ca-rich 3D, Ca-rich 4N1, Ca-rich 4N2. The background marine air particles are labeled: Ca-S 1D, Ca-S 2N, Ca-S 3D, Ca-S 4N. Associated with each particle are volume-equivalent geometric shapes as spheres, spheroids, ellipsoids, cubes, square prisms, rectangular prisms, tetrahedra, and triangular pyramids.

Folders and subfolders contain files associated with:

- Particle compositions by SEM-EDX and volumes of material phases within particles: (*1_Particle_Compositions_Volumes*)
- Spatial and optical parameters for optical modeling of particles and geometric shapes: (*2_Particles_Shapes_Spatial_Optical_Parameters* and subfolders)
- Complex refractive indices for particles and shapes based on Maxwell Garnett average dielectric function: (*3_Complex_RIs_Maxwell_Garnett* and subfolders)
- Results from discrete dipole approximation modeling software DDSCAT ver. 7.3: (*4_DDSCAT_Scattering_Output* and subfolders)
- Mueller scattering matrix elements: (*5_Matrix_Elements* and subfolders)
- Root-mean-square calculations for phase function and degree of linear polarization; (*6_PhaseFunction_LinearPolarization_RMS*)
- Calculations for the backscatter fraction: (*7_Backscatter_Fraction*)

FOLDER CONTENTS

1_Particle_Compositions_Volumes

Composition_MapPointID.xlsx (SEM-EDX analysis results)

Mineral_Al-Si_ratios (Matching of element ratios with compositions of minerals)

Phase_Volumes (Mineral phase volumes from stoichiometric analyses and mineral densities for particles and shapes with ankerite, siderite, and magnetite. Volumes are used in determining particle/shape complex refractive indices from Maxwell Garnett average dielectric function.)

Phase_Volumes_hematite (Mineral phase volumes from stoichiometric analyses and mineral densities for particles and shapes with hematite. Volumes are used in determining particle/shape complex refractive indices from Maxwell Garnett average dielectric function.)

2_Particles_Shapes_Spatial_Optical_Parameters

Dipole_Limit_Calcns.xlsx (Calculations to determine if the number of voxels in particles meets the number of required dipoles for the *mkd* parameter in DDSCAT)

FIB_Avizo_DDA_Input_SizeParameters.xlsx (Input spatial and size parameters, number of dipoles, target origin coordinates for DDSCAT)

Lattice_Spacing_mkd_Calcns_Smoothing.xlsx (Effect of smoothing on lattice spacing and the *mkd* parameter in DDSCAT)

Particle_Axis_Length_Long.xlsx (Determination of long axis for particles)

Spatial_Cross-sectionXYZdistances_AspectRatios.docx (MS Word file with distances in x, y, z directions of particles for determining axes' lengths in geometric shapes and aspect ratios)

Sphere_Spheroid_Ellipsoid_Cube_SqrPrism_RctglPrism.xlsx (Determination of shape parameters for generating geometric shape targets in DDSCAT)

SurfaceArea.xlsx (Determination of surface areas for sphere, prolate spheroid, oblate spheroid, cube, square prism, rectangular prism, tetrahedron, and triangular pyramid)

Subfolders:

Particle_Axis_Length_Data (JPEG and CSV files with particle axis length data based on 3-D projections of particles. Second sub-folder (Original_SE_Images) contains secondary electron images of particles from SEM.)

Spatial_Cross-section_Measurements (JPEG files from Avizo with distance measurements at optimal cross-section planes in particles)

3_Complex_RIs_Maxwell_Garnett

DielectricFunctionsUPDATED.xlsx (Dielectric functions from real and imaginary refractive indices for dolomite, calcite, and gypsum)

Subfolders:

Files within subfolders contain determinations of the lower limit (R_{Imin}) and upper limit (R_{Imax}) to the complex refractive index for particles and associated shapes based on the Maxwell Garnett average dielectric function.

M-G_ExcelFiles_CaMg

M-G_ExcelFiles_Ca-rich

M-G_ExcelFiles_Ca-S

4_DDSCAT_Scattering_Output

DDA_geometric_shape_results_UPDATED.xlsx (Compilation of optical properties – absorption, scattering and backscattering cross sections, asymmetry parameters, backscatter fraction, other properties – and their midpoints for particles and shapes)

DDA_particle_results_UPDATED_smoothed.xlsx (Compilation of optical properties and their midpoints for smoothed particles)

Structure for Subfolder *DDSCAT_files* (raw output):

Within *DDSCAT_files* subfolders are text files containing input parameters (ddscat.par), refractive indices, optical properties for every spatial position and scattering angle for each particle and shape (.sca, .fml), and optical properties in each case averaged over all scattering angles (.avg). Included also are text files with x,y,z coordinates for dipoles within each particle (shape.dat) based on positions of voxels in the 3-D spatial models generated from Avizo. Subfolders contain separate sets of files for runs made with the refractive indices at the lower limit (R_{Imin}) and at the upper limit (R_{Imax}).

1D_CaMg, 2N_CaMg, 3D_CaMg, 4NI_CaMg
ankerite

cube..., ellipsoid..., particle..., pyramid..., rctglprsm..., sphere..., spheroid..., squareprsm..., tetrahdm...

hematite

cube..., ellipsoid..., particle..., pyramid..., rctglprsm..., sphere..., spheroid..., squareprsm..., tetrahdm...

hematite_smoothed

smoothed_level_3

smoothed_level_6

smoothed_level_9

magnetite

cube..., ellipsoid..., particle..., pyramid..., rctglprsm..., sphere..., spheroid..., squareprsm..., tetrahdm...

1D_Ca-rich, 2N_Ca-rich, 3D_Ca-rich, 4N1_Ca-rich, 4N2_Ca-rich

hematite

cube..., ellipsoid..., particle..., pyramid..., rctglprsm..., sphere..., spheroid..., squareprsm..., tetrahdm...

hematite_smoothed

smoothed_level_3

smoothed_level_6

smoothed_level_9

magnetite

cube..., ellipsoid..., particle..., pyramid..., rctglprsm..., sphere..., spheroid..., squareprsm..., tetrahdm...

siderite

cube..., ellipsoid..., particle..., pyramid..., rctglprsm..., sphere..., spheroid..., squareprsm..., tetrahdm...

1D_Ca-S, 2N_Ca-S, 3D_Ca-S, 4N_Ca-S

hematite

cube..., ellipsoid..., particle..., pyramid..., rctglprsm..., sphere..., spheroid..., squareprsm..., tetrahdm...

hematite_smoothed

smoothed_level_3

smoothed_level_6

smoothed_level_9

5_Matrix_Elements

Subfolders: *CaMg, Ca-rich, Ca-S*

Subfolders contain Excel files (*Scattering_Matrix...xlsm*) with scattering matrix elements S11, S12, S21, S22, S31, S41, and the -S12/S11 ratio at angles of theta and phi for the particle, sphere, spheroid, ellipsoid, cube, square prism, rectangular prism, tetrahedron, and triangular pyramid in each case. *CaMg* and *Ca-rich* files show matrix elements from particles and shapes containing the iron phase as iron carbonate, hematite, and magnetite. (Note that Excel files have embedded macros.)

6_PhaseFunction_LinearPolarization_RMS

Files contain the root-mean-square deviations in the geometric shapes from the respective CaMg, Ca-rich, and Ca-S particles for the degree of linear polarization ($-S_{11}/S_{12}$) and the phase function (S_{11}).

LinearPolarization_-S12S11_CaMg_RMS_deviations.xlsx

LinearPolarization_-S12S11_Ca-rich_RMS_deviations.xlsx

LinearPolarization_-S12S11_Ca-S_RMS_deviations.xlsx

PhaseFunction_S11_CaMg_RMS_deviations.xlsx

PhaseFunction_S11_Ca-rich_RMS_deviations.xlsx

PhaseFunction_S11_Ca-S_RMS_deviations.xlsx

7_Backscatter_Fraction

Subfolders: *CaMg, Ca-rich, Ca-S*

Subfolders contain Excel files (*BackscatterFraction...xslm*) with calculations of the backscatter fraction for the particle, smoothed particle, sphere, spheroid, ellipsoid, cube, square prism, rectangular prism, tetrahedron, and triangular pyramid. The backscatter fraction is based on the S_{11} scattering matrix element. (Note that Excel files have embedded macros.)