

Dataset Catalog: Effect of Heterogeneity and Shape on Optical Properties of Urban Dust Based on 3-Dimensional Modeling of Individual Particles

CONTACT

Joseph M. Conny, Ph.D.

joseph.conny@nist.gov

100 Bureau Drive Stop 8372

Gaithersburg, MD USA 20899-8372

DISCLAIMER

This data was developed by employees of the National Institute of Standards and Technology (NIST), an agency of the Federal Government. Pursuant to title 17 United States Code Section 105, works of NIST employees are not subject to copyright protection in the United States and are considered to be in the public domain.

The data is provided by NIST as a public service and is expressly provided "AS IS." NIST MAKES NO WARRANTY OF ANY KIND, EXPRESS, IMPLIED OR STATUTORY, INCLUDING, WITHOUT LIMITATION, THE IMPLIED WARRANTY OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, NON-INFRINGEMENT AND DATA ACCURACY. NIST does not warrant or make any representations regarding the use of the data or the results thereof, including but not limited to the correctness, accuracy, reliability or usefulness of the data. NIST SHALL NOT BE LIABLE AND YOU HEREBY RELEASE NIST FROM LIABILITY FOR ANY INDIRECT, CONSEQUENTIAL, SPECIAL, OR INCIDENTAL DAMAGES (INCLUDING DAMAGES FOR LOSS OF BUSINESS PROFITS, BUSINESS INTERRUPTION, LOSS OF BUSINESS INFORMATION, AND THE LIKE), WHETHER ARISING IN TORT, CONTRACT, OR OTHERWISE, ARISING FROM OR RELATING TO THE DATA (OR THE USE OF OR INABILITY TO USE THIS DATA), EVEN IF NIST HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES.

To the extent that NIST may hold copyright in countries other than the United States, you are hereby granted the non-exclusive irrevocable and unconditional right to print, publish, prepare derivative works and distribute the NIST data, in any medium, or authorize others to do so on your behalf, on a royalty-free basis throughout the world.

You may improve, modify, and create derivative works of the data or any portion of the data, and you may copy and distribute such modifications or works. Modified works should carry a notice stating that you changed the data and should note the date and nature of any such change. Please explicitly acknowledge the National Institute of Standards and Technology as the source of the data: Data citation recommendations are provided below.

Permission to use this data is contingent upon your acceptance of the terms of this agreement and upon your providing appropriate acknowledgments of NIST's creation of the data.

CONTENTS OF DATASET

The dataset consists of Microsoft Excel and Word files, text files, and image bitmap files. The particles are Los Angeles particles 1-4 (LA1-LA4) and Seattle particles 1-3 (S1-S3) as denoted in the file names.

MS Excel files include:

1) Files of calculations for the volumes of the material phases in particles. Note that phase volume calculations were not needed for particles S1 and S3.

LA1_Phase_Volumes
LA2_Phase_Volumes
LA3_Phase_Volumes
LA4_Phase_Volumes
S2_Phase_Volumes_For_Albite_Impurity

2) Files of calculations for approximating the particle complex RIs using the Maxwell-Garnett dielectric function. Note that particle S1 did not require the Maxwell-Garnett approximation.

Maxwell-Garnet_function_calculations\LA1_Maxwell-Garnett_function
Maxwell-Garnet_function_calculations\LA2_Maxwell-Garnett_function
Maxwell-Garnet_function_calculations\LA3_Maxwell-Garnett_function
Maxwell-Garnet_function_calculations\LA4_Maxwell-Garnett_function
Maxwell-Garnet_function_calculations\S2_Maxwell-Garnett_function
Maxwell-Garnet_function_calculations\S3_Maxwell-Garnett_function

3) Files of calculations from the discrete dipole approximation method (DDA) program DDSCAT 7.3 and the dipole limit test.

DDA_Calculations_And_Fractional_Volumes

DDA_Error_Correction_For_Calculations. This file includes systematic computation error as reported in the literature and random error due to the segmentation of particle phases in generating particle 3-D spatial models.

DDA_Dipole_Limit_Test. This file contains information on whether the number of dipoles for each particle meets the criterion for determining scattering efficiencies and the asymmetry parameter as reported in the Draine, B.T. and Flatau, P.J. "User Guide for the Discrete Dipole Approximation Code DDSCAT 7.3, 2013.

MS Word files include:

Particle_Compositions_From_EDX_tabulated.

Particle_Phases_ComplexRIs_Refs_tabulated. This file contains tabulated information on particle phases, volumes of the phases, real and imaginary parts of the complex refractive indexes used for each phase, references for the complex refractive indexes.

Particle_Optical_Properties_tabulated.

Bitmap image files (TIFF and JPEG) include:

1) Scanning electron microscopy (SEM) secondary electron image (SEI) files with electron beam at normal (90°) to the microscope stage or tilted from the stage. The beam energy is either 15kV or 20 kV and the beam current is either 25pA, 580pA, or 620pA as indicated.

LA1\LA1_SEI_5kV_25pA, LA1_SEI_5kV_25pA_tilt60deg

LA2\LA2_SEI_5kV_25pA, LA2_SEI_5kV_25pA_tilt60deg

LA3\LA3_SEI_15kV_580pA, LA3_SEI_15kV_580pA_tilt52deg

LA4\LA4_SEI_15kV_580pA, LA4_SEI_15kV_580pA_tilt52deg

LA4\LA4_slice61_SEI_20kV_620pA. This image is slice no. 61 from the focused ion beam milling process

S1\S1_SEI_20kV_620pA, S1_SEI_20kV_620pA_tilt52deg

S2\S2_SEI_20kV_620pA, S2_SEI_20kV_620pA_tilt52deg

S3\S3_SEI_20kV_620pA, S3_SEI_20kV_620pA_tilt52deg

2) SEM energy dispersive x-ray spectroscopy maps (EDX). Map resolution is 128 x 112.

LA1\EDX_maps\C, O, Si, K, Ca, Ti_ka, Fe_ka

LA2\EDX_maps\C, O, Al, Si, S

LA3\EDX_maps\C, O, Al, S, Fe_ka, Ba_la

LA4\EDX_maps\O, Al, Si, Fe_ka

LA4\EDX_maps\slice61_Al, slice61_Si, slice61_Fe_ka

S1\EDX_maps\O, Na, Al, Si, S, Ca, Fe_ka

S2\EDX_maps\O, Al, Si, S, Ca, Fe_ka

S3\EDX_maps\O, Al, Si, S, Ca, Fe_ka

Text Files

Text files are the input and output files for DDSCAT located in the folder DDA InputOutput Files. Subfolders contain the files for individual particle treatments. For example, under the subfolder for particle S1, the subfolder HOMOSPATIAL Goethite contains the input and output files for the Homogeneous Spatial Model for particle S1 with goethite as the iron oxide phase. The subfolder RCTGLPRSM cube Goethite contains input and output files for the Homogeneous Cubic Model for the same particle. RCTGLPRSM, ELLIPSOID, and TETRHDRN are the DDSCAT target names used in this study for the cubic, spherical, and tetrahedral models.

- The main DDSCAT input parameter file is ddscat.par.
- shape.dat is the input file containing the number of dipoles, the material phases associated with the dipoles and their x,y,z positions in the 3D representations for the Reference Models and Homogeneous Spatial Models.
- px_params xspheres is the file that contains the size of spheres that constitute the Heterogeneous Geometric Models for the LA4 and S3 particle treatments.

- mtable contains the input refractive indexes.
- target.out is the output files from DDSCAT that contains the number of dipoles and their x,y,z positions within the target.
- qtable contains the output scattering efficiencies and asymmetry parameter along with the effective radius of the particle and the incident light wavelength.
- qtable2 contains addition output.