ISSARS Aerosol Database: An Incorporation of Atmospheric Particles into a Universal Tool to Simulate Remote Sensing Instruments

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Abstract

The Instrument Simulator Suite for Atmospheric Remote Sensing (ISSARS) entered its third and final year of development with an overall goal of providing a unified tool to simulate active and passive space borne atmospheric remote sensing instruments. These simulations focus on the atmosphere ranging from UV to microwaves. ISSARS handles all assumptions and uses various models on scattering and microphysics to fill the gaps left unspecified by the atmospheric models to create each instrument's measurements. This will help benefit mission design and reduce mission cost, create efficient implementation of multi-instrument/platform Observing System Simulation Experiments (OSSE), and improve existing models as well as new advanced models in development. In this effort, various aerosol particles are incorporated into the system, and a simulation of input wavelength and spectral refractive indices related to each spherical test particle(s) generate its scattering properties and phase functions. These atmospheric particles being integrated into the system comprise the ones observed by the Multi-angle Imaging SpectroRadiometer(MISR) and by the Multiangle SpectroPolarimetric Imager(MSPI). In addition, a complex scattering database generated by Prof. Ping Yang (Texas A&M) is also incorporated into this aerosol database. Future development with a radiative transfer code will generate a series of results that can be validated with results obtained by the MISR and MSPI instruments; nevertheless, test cases are simulated to determine the validity of various plugin libraries used to determine or gather the scattering properties of particles studied by MISR and MSPI, or within the Single-scattering properties of tri-axial ellipsoidal mineral dust particles database created by Prof. Ping Yang.

I. Introduction

ISSARS provides a universal tool to simulate a wide range of remote sensing instruments. Simulations run within ISSARS are intended to benefit various missions such as the Global Precipitation Measurement(GPM) and Aerosol/Clouds/Ecosystems(ACE) missions[1]. ISSARS employs a web based interface to configure various atmospheric instrument and particle parameters, while a web service is used to perform the computational calculations. These computational calculations are executed in three parts: input reconditioning(IRM), electromagnetic properties(SEAM), and instrument simulation(ISM). This will help benefit mission design and reduce mission cost, create efficient implementation of multi-instrument/platform Observing System Simulation Experiments (OSSE), and improve existing models along with new advanced models being developed[1].

II. ISSARS Computation Flow: IRM, SEAM, ISM

Within the ISSARS's web interface, a user will be able to use a Geophysics/Electromagnetic/Instrument(GEI) interface. This interface will allow the user to fully customize parameters or select a specific list of parameters and constraints already complied based off of existing models or instruments. Once the parameters are selected and submitted, a job number is assigned. The parameters that are submitted are converted and saved as a XML job descriptor file which is used by the IRM[1].

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A. Input Reconditioning Module (IRM)

The geophysics parameters from the job descriptor files are used to determine what source data to utilize. A series of Atmospheric and Surface Model Outputs are also converted into a common format to be used through the remainder of the computation process. These outputs are kept on the same space and time grid of the input models, and contain all the necessary parameters used in the scattering and optical properties calculations. The data found in the XML file determine what data within the Atmospheric and Surface Model Outputs to employ within the space and time grid[1].

B. Scattering/Emission/Absorption Modules (SEAM)

These modules compute various electromagnetic properties of a particle or surface. These are calculated based off on various models such as Rayleigh, Mie, T-matrix[2], and Discrete Dipole Approximation[3]. This stage contains various look up tables(LUT) of pre calculated properties based on a single particle or a volume of particles for a given size distribution. These optical and scattering properties can be a pre-selected by SEAM based on the ranges of the "*particle size vs. wavelength ranges of applicability, or manually by the user*." SEAM will read the grid points generated by the IRM and calculate the electromagnetic properties of the particles and surface. These properties are stored in an identical grid layout as the one used in the IRM output file. The geophysical variables are also processed but are kept separate from the main data to improve memory management[1].

C. Instrument Simulator Modules (ISM)

These modules take in input from the observing geometry, such as the instrument beamwidths, acquisition time, and orbit. Also, the pulse repetition frequency, noise floor, and other instrument characteristics are read and are provided to two modules called the Propagator Module(PM) and the Acquisition Module(AM)[1]. The electromagnetic and geometry grid points created by SEAM constructs an expectation of the signal to be received within the Propagator Module. This module contains Lidar modules, 1-D and 3-D Radiative Transfer(RT) models, Doppler polarimetric radar modules, and the Monte Carlo 3-D polarized Radiative Transfer module. This newly created expected signal is then processed by the Acquisition Module to include output data from the realistic simulation of the instrument from its specific characteristics. This process allows users to test different configurations of the instrument because the data generated by the Propagator Module can be reused to bypass the stages before the ISM. This will greatly increase efficiency within ISSARS. The outputs of this three step process is aerosol and cloud scattering and radiative properties. ISSARS outputs will help in the validation and development of new algorithms of these scattering and radiative properties, as well as retrieval and multi-instrument algorithms[1].

Plugin libraries are also used throughout ISSARS. This libraries store various FORTRAN codes implemented to gather scattering properties of different types of particles. Throughout the three step computational process, these various plugin libraries are run based on the test case selected by the user. These computed properties/values are then used for further calculations or are outputted to the user.

III. The Aerosol Database

With consultation with the MISR team, a list of atmospheric particles were selected to incorporate into ISSARS. Two lists of a spherical particles ranging from spherical marine aerosols to Saharan Dust studied by MISR and MSPI. In addition, a complex database containing various scattering properties created by Prof. Ping Yang[4] is also included in the aerosol database. With a combination of all three data sets within ISSARS, simulations can be run to model various atmospheric particles to obtain the scattering properties.

A. MISR and the MISR Aerosol Dataset

MISR is one of five scientific instruments on the Terra spacecraft. It is orbiting in a polar sun-synchronous orbit around the Earth. This orbit allows MISR to support nine individual cameras that point at different angles in relation to the Earth. These angles are pointed in a way to be beneficial in determining the heights of clouds and terrain, analyzing thermal radiation, and scanning aerosols by looking through maximum atmospheric area[5]. In addition, the orientation of each camera allows the determination of different atmospheric particles due to the change in reflection at different viewing angles. The instrument also provides information to scientists on the partition of energy and carbon in the atmosphere. The nine cameras see in four color bands: red, green, blue, and near infrared. These wavelengths help determine the location of vegetation, reflective properties, and the size and distribution of aerosol particles. This ability to determine different particles in conjunction with stereoscopic techniques allows 3-D models of the total sunlight reflected by Earth's various environments to be constructed. With the use of a database within

ISSARS, the MISR team can help validate existing models on the scattering properties and data collected by their instrument[5].

1. Particle Incorporation into ISSARS

The particles of interest by the MISR team were spherical marine aerosols. The scattering properties of these particles can be determined by Mie code found within SEAMS[2]. The process of incorporating these particles into ISSARS starts with determining how to identify and call upon these particles within ISSARS. This is done by giving each particle a specific identification number. These identification numbers are an eight digit hexadecimal number determined by the particle's chemistry, shape, density, and prolateness ratio. Every particle has its own unique "subkind" identification number. These values are stored within a comma separated value(CSV) file containing the particles specific identification number and the refractive indices of red, green, blue, and near infrared wavelengths.

This CSV file cannot be read directly into ISSARS. This is because the value stored in the CSV file are not in the correct format. Rather than having the values separated by commas, the values need to be separated by tabs. In addition, all values need to be a specific character length. To reformat the existing CSV file, Python is used. Once the conversion is complete, the TSV file is then stored as a plugin library. Plugin libraries are used throughout ISSARS to gather various FORTRAN code to determine numerous scattering properties of the atmospheric particles. This specific plugin libraries uses a FORTRAN code that takes an input of the subkind identification number and frequency, and from the TSV file, generates the real and imaginary refractive indices. This code was also modified to return a linearly interpolated value of the spectral refractive index if the input frequency is not an exact match to the values stored within the TSV file. Once complete, another plugin library is called to run Mishchenko's FORTRAN Mie code to determine the scattering properties of the aerosol particle.

B. MSPI and the MSPI Dataset

MSPI is a multi-directional, multi-wavelength, high-accuracy polarization imager similar to MISR but has some special features that set these two instruments apart. A new camera design is implemented in MSPI to include the ultraviolet and infrared wavelengths not achieved by MISR[6]. The image swath is also larger which allows total global coverage in about 4 days compared to 9 days achieved by MISR[6].

1. Particle incorporation into ISSARS

Like the MISR dataset, the MSPI dataset integrated for ISSARS' aerosol database. The MSPI dataset is composed of mineral aerosol particles and the list contains the frequency, and the real and imaginary refractive indices for 1% and 3% hematite content. The shape distributions are based on Saharan Mineral Dust Experiment(SAMUM). These particles are fitted with four-modal lognormal distribution with the radius ranging from 0.05 to 10um[7]. Figure 1 displays the shape distribution based on SAMUM. Different shape distributions over a range of size intervals are given in Fig. 1. It is important to note that a particle's radius less than 0.25µm shows a decreasing trend as aspect ratio increases. In addition, the shape distribution for particles greater than 0.5µm follows the same decreasing trend, but these distributions are different than seen for small particles. These two shape distributions create a transition region between 0.25-0.5µm, so two test cases can be used within the T-matrix calculations. One test case is particle less than 0.35µm and the other is particles greater than 0.35µm. These distributions are averaged over the aspect ratio range with a median aspect ratio of 1.3 and 1.65 for small and large particles respectivley[7]. A summary of the values used within the T-matrix calculations based off of Fig. 1 is shown in Table 1.

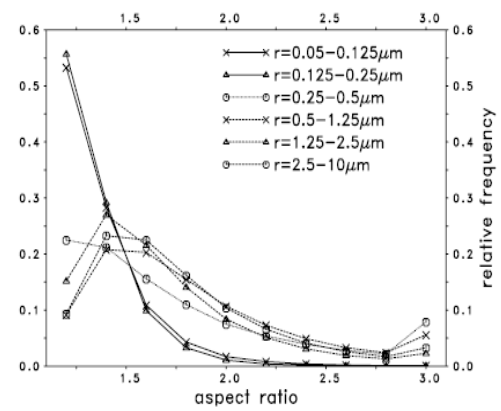

Figure 1. *Shape distribution over a range of size intervals(0.05-10µm). From Wiegner, M., and Gasteiger, J.*

To incorporate the MSPI aerosol particles into ISSARS, two separate plugin libraries were created. One dust absorption with 3% hematite and one dust absorption with 1% hematite. A Fortran code found within these libraries will return the real and imaginary refractive indices based on an input frequency. Unlike the MISR plugin library, these two MSPI libraries do not use a TSV file to obtain the appropriate values based on user input due to a small range of wavelengths and refractive indices. Instead, all data is stored in arrays within the Fortran code implemented in these libraries. All values for the refractive indices returned will either be an exact match or a linear interpolation

based on how exact the input frequency is to the ones stored within the code. To control how exact the input frequency has to be to return an exact matched refractive index, a tolerance within the FORTRAN code is also use. This can be changed in the future to determine if a input frequency is "exact". Subkind identification numbers are also given to these particles. These numbers are based on the aspect ratio range and corresponding frequency found in Table 1. ISSARS will read these subkind identification numbers selected by the user to run in the T-matrix. Once complete, the scattering properties and phase matrix values will be returned.

Table 1: ***List of frequencies(μm) for the two test cases described in SAMUM as aspect ratio increases. From Wiegner, M., and Gasteiger, .***

ε'	$r < 0.35\,\mu m$	$r > 0.35\,\mu m$
1.2	0.535	0.103
1.4	0.289	0.234
1.6	0.108	0.218
1.8	0.040	0.157
2.0	0.015	0.101
2.2	0.007	0.065
2.4	0.003	0.041
2.6	0.001	0.027
2.8	0.001	0.018
3.0	0.001	0.036

C. Professor Ping Yang's Single-scattering Properties of Tri-axial Ellipsoidal Mineral Dust Particles Database

This database is a massive collection of single-scattering properties based upon predetermined microphysical and optical parameters[4]. These single-scattering properties of the single dust particle are the extinction efficiency, single-scattering albedo, and phase matrix; hence, the predetermined parameters used to determine these scattering properties are the size aspect ratio, real and imaginary refractive indices, size parameter, and scattering angles. Table 2 gives a list of the predetermined parameters within Prof. Ping Yang's Database. Each database is stored as a .nc file containing the file format "Database_yx%.2f_zx%.2f_mr%.2f_mi%.4f.nc". Based off of Table 2, only a hand full of combinations are present within the database. This leads to 420 files within the database which correspond to 15 shapes and 28 sets of refractive indices. These types of particles range from spheres to prolate, oblate, and tri-axial ellipsoids. The microphysical parameters of the participles are also fixed. Figure 2 displays an overview of how Prof. Ping Yang's Database is structured. The single scattering properties found within this database can be used to find the bulk scattering properties of an ensemble of aerosol particles. However, according to Prof. Ping Yang, it is:

> *quite challenging to accurately simulate backscattering and the present database is more suitable in terms of accuracy for passive remote sensing based on satellite observations than it is for lidar studies*[4].

Table 2. Possible values used within Ping Yang's database when describing the predetermined values.

έ	mr	mi
1.00	1.10	0.0005
1.02	1.20	0.001
1.05	1.30	0.005
1.10	1.40	0.01
1.13	1.50	0.02
1.16	1.60	0.05
1.20	1.70	0.08
1.50	1.90	0.1
1.80	2.10	0.2
2.10		0.5
2.40		
2.70		
3.30		

1. Incorporation of Professor Ping Yang's Database into ISSARS

The overall procedures for incorporating this library into ISSARS is a little different than the first two mentioned. The same structured plugin library was created but the FORTRAN code is used to extract data from a specific database based on user input of the prolateness ratio, real and imaginary refractive indices, radius of particle, frequency, and scattering angles of interest. This plugin library extracts data from the databases representing spheres and prolate/oblate ellipsoids only. Tri-axial ellipsoids have a special plugin library created. Since there is only so many possible combinations that this database could have based on the pre determined aspect ratios and real and imaginary refractive indices, ISSARS will give a warning to the user that the closest possible combination of values were chosen. If a user diverges from the possible combination of these values, this will give the user the ability to abort the simulation, continue with the new values, or access a web page and input an exact value found in this database to run the simulation.

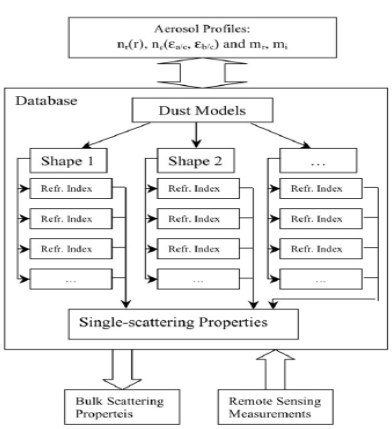

Figure 2. *Layout of how Ping Yang's database* structured and can be used. From Meng, Z.,Yang, P., Kattawar, G. W.,Lei, B., Liou, K.N., and Laszlo I.

All of Prof. Ping Yang's databases will be stored in ISSARS. Once a database is selected within ISSARS, all of the scattering properties and phase matrix values are read using NetCDF. The values within the database are stored as a 3-D matrix. The first dimension is the size parameter. These size parameters are logarithmically distributed between 0.025 and 1000^3. The second dimension is the scattering angles from 0-180 degrees. There are 500 different angles stored within Prof. Ping Yang's Database. The third dimension stores the phase matrix values corresponding to ln(P11),P12,P22,P33,P34, and P44, the only non-zero elements of the phase matrix for randomly oriented particles. Desired values from the 3-D matrix is gathered based on the user inputs. The FORTRAN code will convert the inputs into the corresponding size parameter. Based on this value determined, the FORTRAN code will either gather an exact readout of the scattering properties or a linear interpolated value of these properties. The same process is done with the scattering angles. Based off of how exact the angles are compared to the values found within the database, the FORTRAN code will return the exact values or the linear interpolated values of the phase matrix.

IV. Testing and Results

A. MISR Testing

Graphing the trend to see how the refractive indices vary with frequency was one way to test the validity of the FORTRAN code used to extract the correct values from the TSV file. For the real part of the refractive index, the values do not change for each aerosol particle as the frequency is increased. However, graphing the imaginary refractive index displays a linear trend. Figure 3 displays all four refractive indices within the MISR Aerosol database for a spherical absorbing sulfate particle at different effective radii. One will note that the imaginary refractive index decreases or increases. This is why a linear interpolation is introduced into the code for unknown test frequencies. To verify the code is correctly determining a linear interpolation of the refractive indices, a Python module was used to acquire the refractive indices at various frequencies ranging from blue to near infrared wavelengths. Figure 4 displays these results.

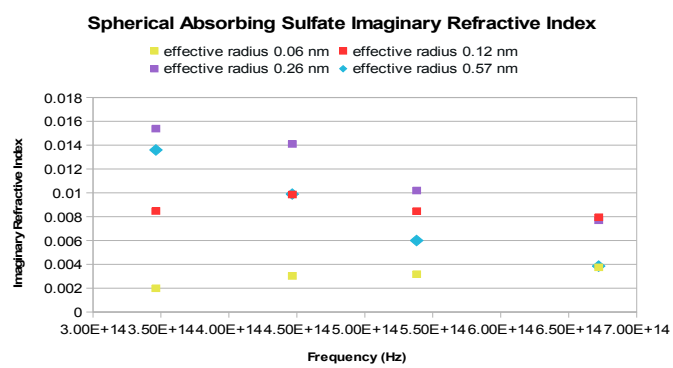

Figure 3. *Imaginary refractive indices given a range of radius for a spherical absorbing sulfate aerosol.*

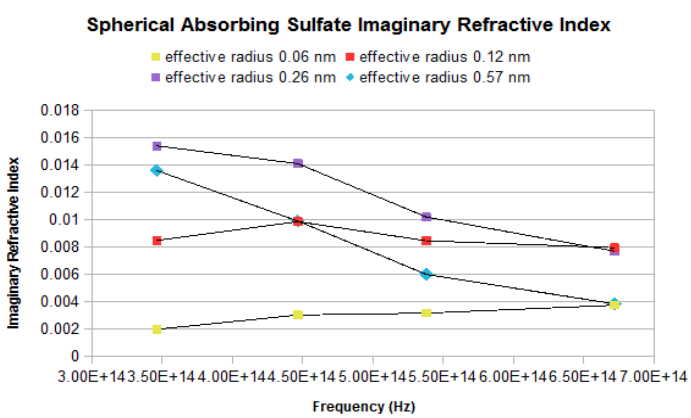

Figure 4. *Validation test to determine if linear interpolation is working.*

B. MSPI Testing

These particles were tested in the similar way as the MISR particles. Both cases of dust absorption (1% and 3% hematite) were tested. Figure 5 shows the imaginary refractive indices of these dust absorptions at the frequencies given by the MSPI team. It is clear by this figure that a linear regression of the whole set is not good for determining unknown refractive indices; however, a linear interpolation is adequate between successive samples since there is not an efficient model to represent the refractive indices at different frequencies. Plotting the frequency at different values, as shown in Fig. 5, will help determine if the code is working correctly. This figure can verify that between two points, the imaginary refractive indices are the interpolated linearly.

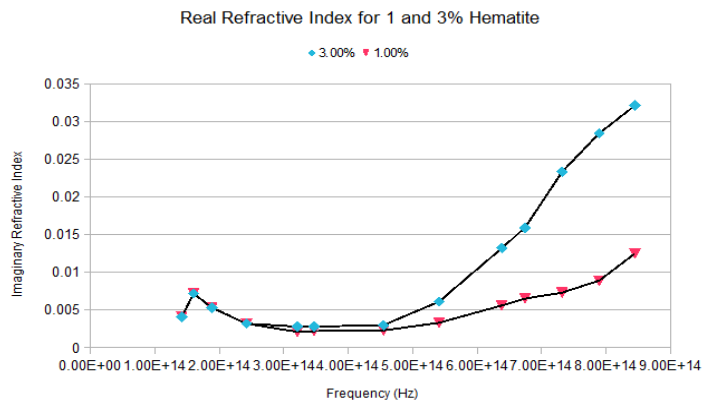

Figure 5. *Imaginary refractive indices for a range of frequency for 1 and 3% hematite.*

The FORTRAN codes found in these particular plugin libraries returns a "status" value that clarifies to the user that the returned values of the refractive indices are interpolated, an exact value found in the dataset, or the test was unsuccessful. A tolerance check within the code is also implemented. This check makes it possible to return a "status" value of "exact match" even though the input frequency was not an exact match found in the dataset. By increasing the tolerance check/value to a extremely high value, a test case will show if the tolerance is working. Figure 6 and 7 shows tests for 3% and 1% hematite, respectively. A zero slope at every exact point within the dataset is shown in the graph. This verifies that the tolerance check, extremely exaggerated in these test cases, is working correctly.

C. Professor Ping Yang's Single-scattering Properties of Tri-axial Ellipsoidal Mineral Dust Particles Database Testing

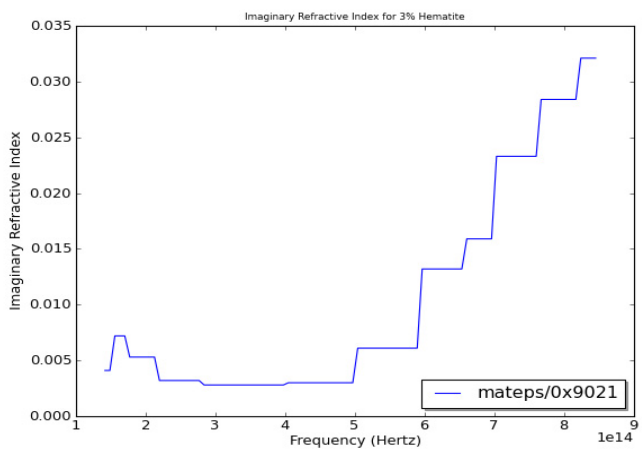

Figure 6. *Validation test of 3% hematite to determine if tolerance within code is working.*

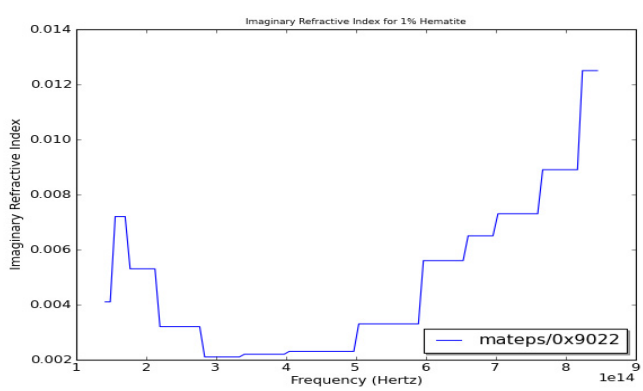

Figure 7. Validation test of 1% hematite to determine if tolerance within code is working.

Prof. Ping Yang's database was tested for spherical particles. Graphing the results of the extinction and scattering cross section area, and asymmetry parameter over a range of the particles radius; thus, comparing these results with the extinction and scattering section area, and asymmetric parameters generated with Mie code will determine if a linear interpolation is valid for unknown parameters. Figure 7 shows the trend of Prof. Ping Yang's results with Mie codes results at a frequency of 446.4ηm. One will notice that linear interpolation within the code is working. Plus, the black squares show the point where Prof. Ping Yang's database gives an exact value for the scattering properties. For small particles, the linear interpolation within Prof. Ping Yang's Database is consistent with the Mie code. As the test particle gets larger, there is a divergence with how exact Prof. Ping Yang's database compared to Mie code. This could be because Prof. Ping Yang used a different computational method for larger particles. Along with Mie code, an improved geometric optics method(IGOM) was used for particles whose size parameters range from 10-1000[4]. This could have caused the values of Prof. Ping Yang's database to not be consistent with the Mie code. Figure 8 also show the back scattering cross section area generated by Prof. Ping Yang's database and Mie code. Again, smaller radius values

used generated an overall agreeable result that gets worse as the particles radius gets larger. However, Figure 9 show the asymmetric parameter is agreeable no matter how large the particle is.

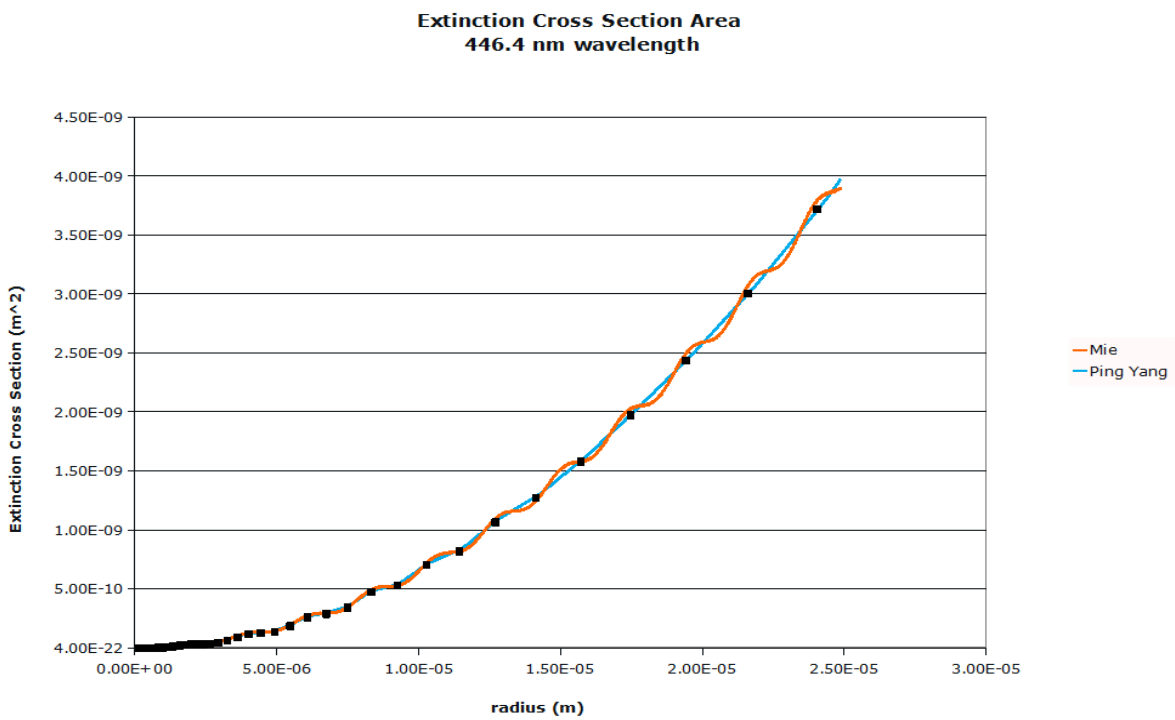

Figure 7. *Mie and Ping Yang's database results for the extinction cross section area as the test particle's radius increase.(constant 446.4nm wavelength)*

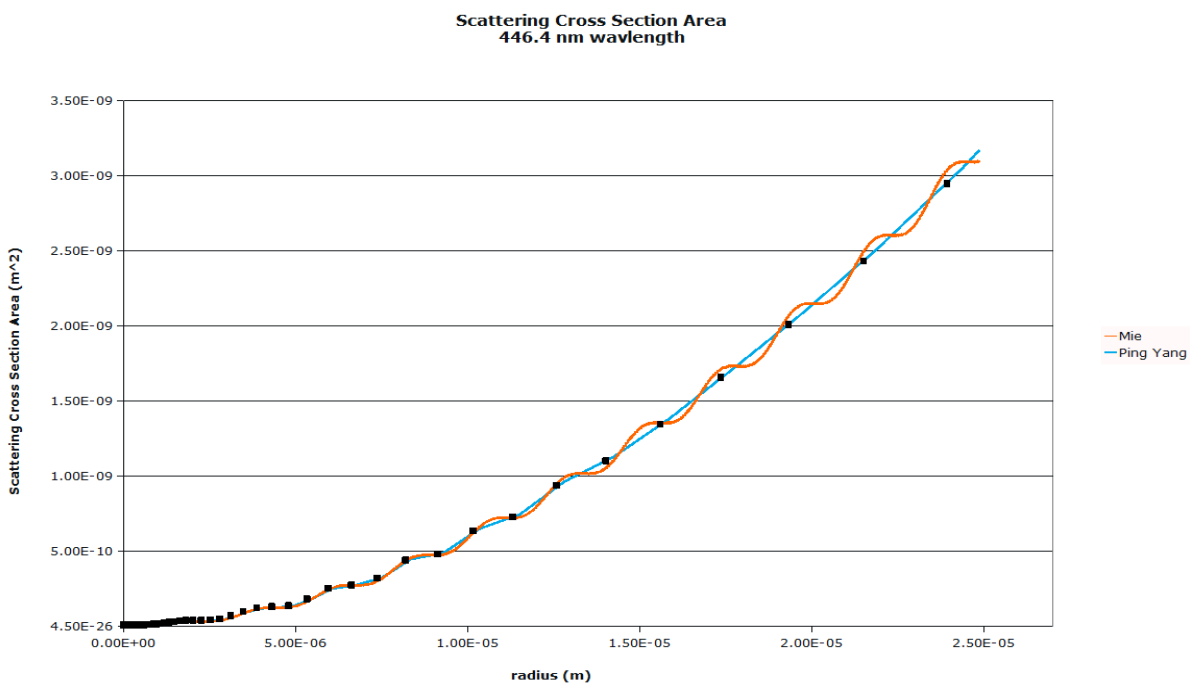

Figure 8. *Mie and Ping Yang's database results for the scattering cross section area as the test particle's radius increase.(constant 446.4nm wavelength)*

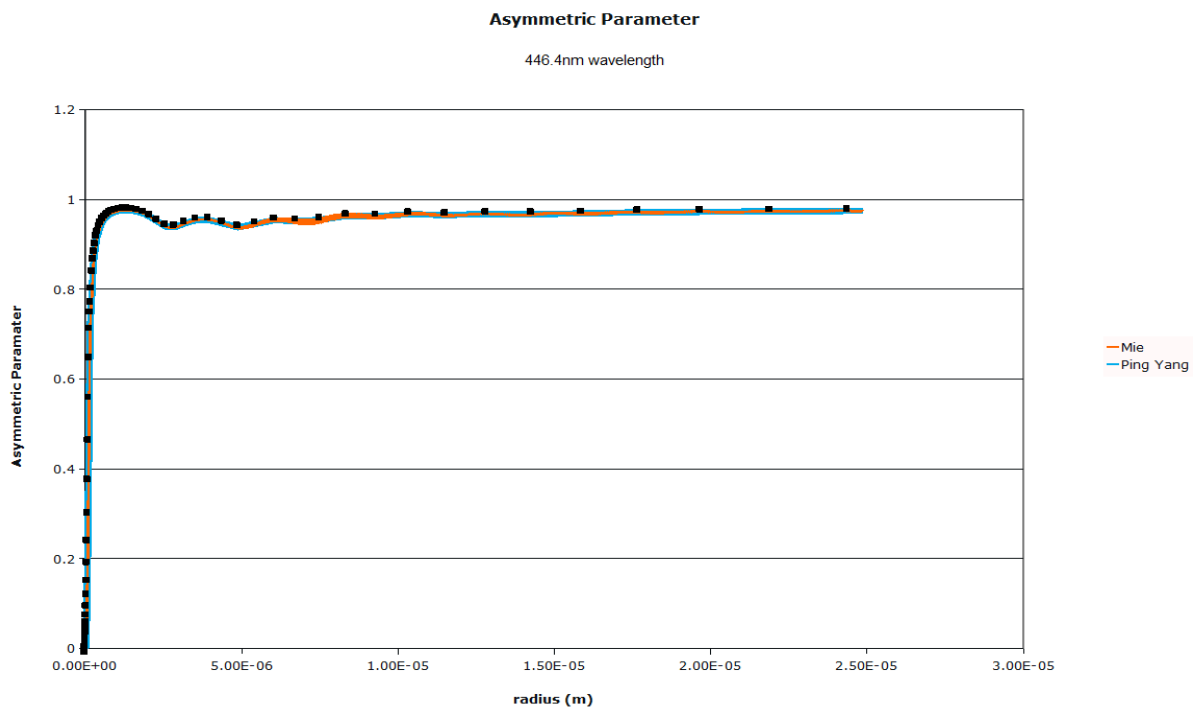

Figure 9. *Mie and Ping Yang's database results for the asymmetric parameter as the test particle's radius increase.(constant 446.4nm wavelength)*

V. Conclusion

Future testing with more particles is still needed. For the MISR particles, the generated outputs of the real and imaginary refractive indices still need to be used with the Mie code found within SEAM to test the validity of the results. In addition, testing prolate and oblate particles needs to be done with Prof. Ping Yang's database to test if linear interpolation is enough for unknown ranges of size, wavelength, and scattering angles not present in the database. Future analysis with these tests can also determine if ISSARS can be used to generate the scattering properties and phase matrix for MSPI particles in the database. This will allow a combination of both plugin libraries to be used for the MSPI particles whose return values are not present with the aerosol database.

Acknowledgments

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References

[1]Tanelli, S., and Tao, W., and Hostetler, C., "NASA's integrated Instrument Simulator Suite for Atmospheric Remote Sensing from spaceborne platforms(ISSARS) and its role for the ACE and GPM missions," *Earth Science Technology Office* [online article], URL: http://esto.nasa.gov/conferences/estf2011/papers/Tanelli_ESTF2011.pdf.

[2]Mishchenko M. I, "Scattering, Absorption, and Emission of Light by Small Particles", Cambridge University Press, Cambridge (2002).

[3]Yurkin M.A., Maltsev V.P., and Hoekstra A.G., 2007: The discrete dipole approximation for simulation of light scattering by particles much larger than the wavelength. Journal of Quantitative Spectroscopy and Radiative Transfer 106, 546–557.

[4]Meng, Z.,Yang, P., Kattawar, G. W.,Lei, B., Liou, K.N., and Laszlo, I., "Single-Scattering properties of tri-axial ellipsoidal mineral dust aerosols: A database for application to radiative transfer calculations," *Journal of Aerosol Science 41 (2010) 501-512* URL: http:/www.elsevier.com/loacate/jaerosci.

[5]"MISR Instrument." *MISR: Multi-angle Imaging SpectroRadiometer*. JPL, n.d. Web. 6 Sep 2011. <http://www-

misr.jpl.nasa.gov/Mission/misrInstrument/>.

[6]"AirMSPI." *Airborne Multiangle SpectroPolarimeter Imager*. JPL, n.d. Web. 6 Sep 2011. <http://airbornescience.jpl.nasa.gov/airmspi/>.

[7]Wiegner, M., and Gasteiger, J. "Numerical simulations of optical properties of Saharan dust aerosols with emphasis on lidar applications," *International Metrological Institute in Stockholm* [online article],Tellus: Series B Chemical and Physical