Optimization of aerosol parameters to achieve the greatest possible microwave attenuation

User manual to the program "attenuation.exe"

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1. Introduction

The program "attenuation.exe" is used to find the optimal parameters of dust to achieve the greatest possible attenuation in the microwave frequencies. The program tests all combinations of the following parameters:

- Microwave frequency
- The real part of the refractive index of particles
- The imaginary part of the refractive index of the particles
- The radius of dust particles (monodisperse aerosol)
- Dust particle temperature
- The surface potential of dust particles
- The proportionality coefficient in relation (14) in the theoretical description of the calculation method (fixed value)

Each parameter is tested in a range of values from a selected interval, and the user can set:

- Minimum value
- Maximum value
- Number of values between the maximum and the minimum
- Linear or logarithmic scale of values within an interval

For each parameter combination, the program calculates the attenuation and saves the results in an output file for further processing. Due to the huge number of combinations, the output file can be difficult to process (for example, MS EXCEL can handle a maximum of about 1,000,000 lines). Therefore, the user can set how many best parameter combinations for one frequency should be stored (for example, if the value 1 is chosen, only the most advantageous parameter combination will be saved).

The program can test about 50,000 combinations of parameters per second on a standard "office" PC.

2. Program inputs

2.1. Command line parameters

The "attenuation.exe" program reads the inputs from the configuration file. The name of the configuration file is the first command line parameter of the program.

Example:

attenuation.exe testconfig.txt - the program reads the parameters from the file
"testconfig.txt"

In the MS Windows environment, the user can simply throw the "testconfig.txt" file into the "attenuation.exe" program using the mouse.

2.2. Structure of the configuration file

The configuration file contains lines with keywords (they are written in capital letters below). These lines contain configuration parameters. All other lines are ignored and can be used as a comment. The only exceptions are the lines after the keyword "MATERIALS", which are understood as file names (more details below).

FREQUENCY <smallest value> <largest value> <number of values> <scale>

This line specifies the frequency values in GHz to be tested. The scale can be LIN (linear) or LOG (logarithmic) and determines the distribution of values between the smallest and largest value.

Examples:

FREQUENCY 10 100 10 LIN -10 values evenly distributed between the smallest and the largest value are tested, including 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 GHz

```
FREQUENCY 30 30 1 LIN — a single 30 GHz value is tested

FREQUENCY 1 100 3 LOG — the values of 1, 10, and 100 GHz are tested

FREQUENCY 20 30 2 LIN — 20 and 30 GHz values are tested
```

The frequency has special importance during testing – at least one value of the (largest) attenuation for each tested frequency is always stored in the output file. The range of frequency values is allocated dynamically; there is no restriction on the number of frequencies.

RADIUS <smallest value> <largest value> <number of values> <scale>

This line specifies the particle radius values in micrometers. The parameter values have the same meaning as for "FREQUENCY".

Example:

```
RADIUS 0.001 1000 600 LOG — 600 values with logarithmic distribution are tested, i.e., 100 values between 0.001 and 0.01, 100 values between 0.01 and 0.1, etc.
```

The range of radius values is allocated dynamically; there is no restriction on the number of radii.

REFR_INDEX_REAL <smallest value> <largest value> <number of values> <scale>

This line specifies the values of the real part of the refractive index of the particles to be tested. The parameter values have the same meaning as for "FREQUENCY".

Example:

```
REFR_INDEX_REAL 1 5 9 LIN — 9 evenly distributed values between 1 and 5 will be tested: 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5 and 5.
```

The range of the values of the real part of the refractive index is allocated dynamically; there is no restriction on the number of values.

REFR_INDEX_IMAG <smallest value> <largest value> <number of values> <scale>

This line specifies the values of the imaginary part of the refractive index of the particles to be tested. The parameter values have the same meaning as for "FREQUENCY".

Example:

```
REFR_INDEX_IMAG 0 2 11 LIN — 11 values will be tested: 0.0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8 and 2.0
```

The range of the values of the imaginary part of the refractive index is allocated dynamically; there is no restriction on the number of values.

MATERIALS < number of materials >

This is an alternative way of finding the most suitable particle material. Instead of searching for the most suitable refractive index, the most suitable material from the list following this line is searched. The following <number of materials> lines are understood to be the names of the files containing the wavelength dependence of the refractive index. Blank lines are ignored.

Example:

```
MATERIALS 2
maroko_burka_n.dat
mediterian n.dat
```

It is testing two materials whose refractive indices are listed in the files "maroko_burka_n.dat" and "mediterian_n.dat".

The number of files and refractive index values are allocated dynamically; there is no restriction on the number of files or the number of refractive index values.

The "MATERIALS" parameter has higher priority than the "REFR_INDEX_REAL" and "REFR_INDEX_IMAG" parameters. If the number after "MATERIALS" is greater than zero, the lines "REFR_INDEX_REAL" and "REFR_INDEX_IMAG" are ignored. Conversely, if zero material ("MATERIALS 0") is specified, any file names in the following lines are ignored and the values of the real and imaginary parts of the refractive index are tested (the "REFR_INDEX_REAL" and "REFR_INDEX_IMAG" parameters are used).

Wavelength-dependent files with a refractive index dependence (n '- i * n' ') are compatible with the "visibility.exe" program, i.e.:

- Lines beginning with '#' are ignored (comments)
- There are 3 positive values in each line: <wavelength in micrometers> <real part of the refractive index> <imaginary part of the refractive index>
- Wavelengths are listed in ascending order from smallest to largest
- If the refractive index for a wavelength is not specified in the file, the following is used : o The linearly interpolated value between the two closest, if available

- o The value for the smallest wavelength specified in the file (if the required wavelength is lower)
- o The value for the largest wavelength specified in the file (if the required wavelength is higher)

TEMPERATURE <smallest value> <largest value> <number of values> <scale>

This line specifies the temperature values of the particles in Kelvin (relation (16) in the theoretical part). The parameter values have the same meaning as for "FREQUENCY".

Example:

```
TEMPERATURE 300 300 1 LIN -1 value is tested: 300 K
```

The range of temperature values is allocated dynamically, there are no restrictions on the number of values.

POTENTIAL <smallest value> <largest value> <number of values> <scale>

This line specifies the values of the particle surface potential in volts (relation (15) in the theoretical part) to be tested. The parameter values have the same meaning as for "FREQUENCY".

Example:

```
POTENTIAL 0 100 2 LIN -2 values are tested: 0V a 100V
```

The range of the surface potential values are allocated dynamically, there are no restrictions on the number of values.

COEFF <value>

This line determines the value of the proportionality coefficient in relation (16) in the theoretical part. The value is in the range of 0.1 - 10, and the recommended value is 1.

Example:

```
COEFF 1.0 — the value 1.0 is used
```

SHOW_BEST < value>

This line determines how many combinations of parameters with the highest attenuation are stored in the output file.

Examples:

```
SHOW_BEST 0 — all combinations are saved (the file can be huge)

SHOW_BEST 1 — one combination with the highest attenuation for each frequency is stored

SHOW_BEST 100 — one hundred combinations with the highest attenuation for each frequency are stored
```

2.3 Constant parameters

Attenuation is calculated for a fixed aerosol volume concentration of 1 cm³/1m³. At a material density of, for example, 2.7 g/cm³, which corresponds to a mass concentration of 2.7 g/m³. The attenuation is directly proportional to the volume concentration of the particles: at a 10x lower

concentration, it will be 10x smaller (and vice versa). This makes it easy to determine the concentrations required to achieve the desired attenuation.

3. Program outputs

The "attenuation.exe" program saves the results in the "attenuation.dat" file. In each row, the following values are stored in each column:

- Frequency in GHz
- Material refractive index file name (if MATERIALS> 0)
- The real part of the refractive index
- The imaginary part of the refractive index
- Radius of particles in micrometers
- Temperature in Kelvin
- Potential in Volts
- Attenuation in dB/km

Depending on the value of the "SHOW_BEST" parameter, only the corresponding number of parameter combinations leading to the highest attenuation is stored for each frequency.

The file "attenuation.dat" uses a tab as a column separator, compatible with spreadsheets, such as MS EXCEL. Depending on the default language settings of the operating system, it may be necessary to replace all decimal points in the numbers in the "attenuation.dat" file with decimal points.

Example of part of the "attenuation.dat" file:

30	maroko_burka_n.dat	2.584	0.03205	7.17E-01	300	92	1.422
30	maroko_burka_n.dat	2.584	0.03205	7.47E-01	300	100	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.97E-01	300	87	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.81E-01	300	83	1.422
3.0	maroko burka n.dat	2.584	0.03205	6.43E-01	300	74	1.422

Illustrations of how to use the "attenuation.dat" file for various analyses are given in the appendices below.

Appendix 1. Verification of computations

Appendix 1.1. Rayleigh approximation

Verifying that the program calculates the attenuation in the long-wave regime correctly (the wavelength of the radiation is much larger than the particle size) the proportionality to the fourth-square of the frequency was tested. The frequency range of 0.1 – 100 GHz for a non-charged particle of size 10 μ m with the refractive index of n = 2.0-0.0i was tested. Input parameters for "attenuation.exe":

```
FREQUENCY 0.1 100 100 LOG

MATERIALS 0

REFR_INDEX_REAL 2.0 2.0 1 LIN

REFR_INDEX_IMAG 0.0 0.0 1 LIN

RADIUS 10 10 1 LIN

TEMPERATURE 300 300 1 LIN

POTENTIAL 0 0 1 LIN

COEFF 1

SHOW_BEST 0
```

Figure 1 shows the dependence of attenuation on the frequency on a logarithmic-logarithmic scale. The obtained linearly proportional dependence of the attenuation on the fourth-square of the frequency is obvious. Using the least-squares method confirmed that it is a power of the fourth-order. This means that the program calculates the extinction coefficient and the attenuation in the long-wave regime for the uncharged particles correctly.

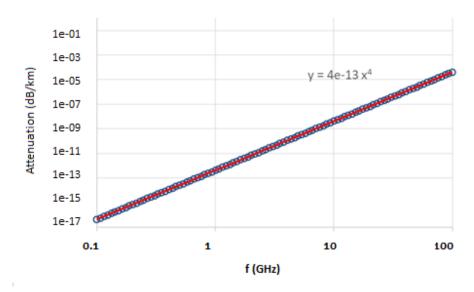


Fig. 1. Dependence of attenuation on frequency. The red line corresponds to the least-squares fitting method.

Appendix 1.2. Mie resonances

Verification that the program calculates the resonant attenuation at a particle size comparable to the wavelength is shown. We use a frequency of 100 GHz (wavelength of 3 mm) and a particle size of 100 - 100,000 μ m (0.1 - 100 mm). Input parameters for "attenuation.exe":

```
FREQUENCY 100 100 1 LOG
MATERIALS 0
REFR_INDEX_REAL 2.0 2.0 1 LIN
REFR_INDEX_IMAG 0.0 0.0 1 LIN
RADIUS 1e2 1e6 400 LOG
TEMPERATURE 300 300 1 LIN
POTENTIAL 0 0 1 LIN
COEFF 1
SHOW_BEST 0
```

Figure 2 shows a series of significant maximum attenuation at the particle sizes comparable to the wavelength, as shown by the Mie theory. The left part of the graph for small particle sizes shows the power dependence of the attenuation on the particle size, which corresponds to the analogous dependence on the frequency at a constant particle radius analyzed in Appendix 1.1.

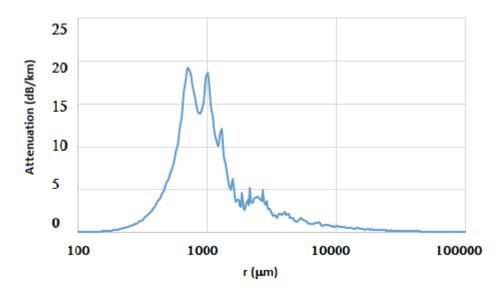


Fig. 2. Dependence of attenuation on particle radius

Appendix 1.3. Surface charge resonances

To verify that the program calculates the resonant attenuation caused by the surface charge correctly, we model the same situation as published in the article (Kocifaj, 2016). Calculation of the ratio of extinction coefficients (identical to the attenuation ratio - relations (17) and (19) in the theoretical part) was compared. The charged (5V potential) and uncharged particles at the frequency of 6,000 GHz, temperature 100 K, and different particle sizes were tested. The particle size is characterized by the size parameter x (relation (2) in the theoretical part). The refractive index has a value of 1.93 - 0.037 i. Input parameters for "attenuation.exe":

```
FREQUENCY 6000 6000 1 LOG
MATERIALS 0
REFR_INDEX_REAL 1.93 1.93 1 LIN
REFR_INDEX_IMAG 0.037 0.037 1 LIN
RADIUS 1e-3 10 400 LOG
TEMPERATURE 100 100 1 LIN
POTENTIAL 0 5 2 LIN
COEFF 1
SHOW BEST 0
```

The processed "attenuation.dat" file (with the calculated size parameter x and determined attenuation ratio at 5V and 0V potentials) is shown in Figure 3, which documents the accuracy of the calculation with the article (Kocifaj, 2016).

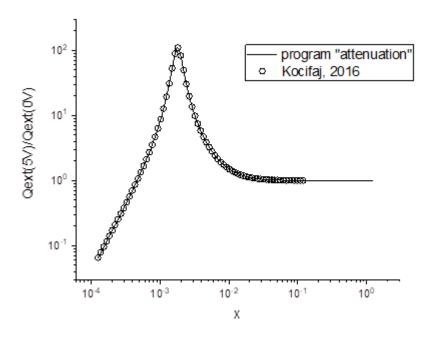


Fig. 3. Comparison of the "attenuation.exe" calculation with data from the article Kocifaj, 2016

Appendix 2. Examples of particle optimization

Appendix 2.1. Particle refractive index optimization

In the long-wave regime, at the frequency of 30 GHz, the particle radii $0.1-100~\mu m$, the real part of the refractive index 1.0-5.0 and the imaginary part of the refractive index 0.0-4.0 were tested (a total of about 300,000 combinations). The 500 most advantageous combinations of parameters were stored. The optimal refractive index of particles with the highest attenuations was found as follows:

Input parameters for "attenuation.exe":

```
FREQUENCY 30 30 1 LOG
MATERIALS 0
REFR_INDEX_REAL 1 5 101 LIN
REFR_INDEX_IMAG 0.0 4.0 101 LIN
RADIUS 0.1 100 30 LOG
TEMPERATURE 300 300 1 LIN
POTENTIAL 0 0 1 LIN
COEFF 1
SHOW_BEST 500
```

First lines of the file "attenuation.dat":

f[GHz]	mater.	maal (n)	imag(n)	m [mlem]	+om [K]	not [37]	att.[dB/km]
30	-	rear(n)	1.44	100	300	0	7.761
30	_	1	1.44	100	300	0	7.755
30	_	1	1.44	78.8	300	0	7.748
30	_	1	1.48	78.8	300	0	7.741
30	_	1	1.44	62.1	300	0	7.741
30	_	1	1.4	100	300	0	7.738
30	_	1	1.44	48.94	300	0	7.736
30	_	1	1.48	62.1	300	0	7.733
30	_	1	1.44	38.57	300	0	7.733
30	_	1	1.44	30.39	300	0	7.731
30	_	1	1.44	23.95	300	0	7.73
30	_	1	1.44	18.87	300	0	7.729
30	_	1	1.44	14.87	300	0	7.729
30	_	1	1.44	11.72	300	0	7.728
30	_	1	1.44	9.237	300	0	7.728
30	_	1	1.44	7.279	300	0	7.728
30	_	1	1.44	5.736	300	0	7.728
30	_	1	1.48	48.94	300	0	7.728
30	_	1	1.44	4.52	300	0	7.728
30	_	1	1.44	3.562	300	0	7.728
30	_	1	1.44	2.807	300	0	7.728
30	_	1	1.44	2.212	300	0	7.728
30	_	1	1.44	1.743	300	0	7.728
30	_	1	1.44	1.374	300	0	7.728
30	_	1	1.44	1.083	300	0	7.728
30	_	1	1.44	0.8532		0	7.728
30	_	1	1.44	0.6723		0	7.728
30	_	1	1.44	0.5298		0	7.728
30	_	1	1.44	0.4175		0	7.728
30	_	1	1.44	0.329	300	0	7.728
30	_	1	1.44	0.2593		0	7.728
30	_	1	1.44	0.2043		0	7.728
30	_	1	1.44	0.161	300	0	7.728

```
30
            1.44 0.1269 300 0
                               7.728
30
            1.44 0.1 300 0
                               7.728
30
       1
            1.4 78.8 300 0
                               7.727
30
            1.48 38.57 300 0
       1
                               7.725
30
        1
            1.48 30.39 300 0
                               7.723
30
        1
            1.48 23.95 300 0
                               7.722
        1
30
             1.48 18.87 300 0
                               7.721
```

The highest attenuation of about 7.7 dB/km is achieved for the real part of the refractive index equal to 1.00 and the imaginary part of the refractive index equal to 1.44, while it practically does not depend on particle size (their volume in 1m³ is constant in calculation and does not depend on particle radius). Of course, we probably cannot find a material with such a refractive index, but we should look for a material with properties as close as possible.

Appendix 2.2. Particle radius optimization

The optimal particle radius for the frequency of 100 GHz was found. Testing particle radii of $0.1 - 1000 \, \mu m$ using a refractive index of 2.0 - 0.00 i (typical lossless dielectric material) were used.

Input parameters for "attenuation.exe":

```
FREQUENCY 100 100 1 LOG
MATERIALS 0
REFR_INDEX_REAL 2 2 1 LIN
REFR_INDEX_IMAG 0 0 1 LIN
RADIUS 0.1 1000 4000 LOG
TEMPERATURE 300 300 1 LIN
POTENTIAL 0 0 1 LIN
COEFF 1
SHOW_BEST 100
```

First lines of the file "attenuation.dat":

f[GHz]	mater.	real(n)	imag(n)	r[mkm]	tem.[K]	pot.[V]	att.[dB/km]
100	_	2	0	716.1	300	0	19.24
100	-	2	0	714.4	300	0	19.24
100	-	2	0	717.7	300	0	19.24
100	-	2	0	712.8	300	0	19.24
100	-	2	0	719.4	300	0	19.23
100	-	2	0	711.2	300	0	19.22
100	-	2	0	721	300	0	19.22
100	-	2	0	709.5	300	0	19.21
100	-	2	0	722.7	300	0	19.2
100	-	2	0	707.9	300	0	19.18
100	-	2	0	724.4	300	0	19.17
100	-	2	0	706.3	300	0	19.15
100	-	2	0	726	300	0	19.14
100	-	2	0	704.6	300	0	19.12
100	-	2	0	727.7	300	0	19.11
100	-	2	0	703	300	0	19.07
100	-	2	0	729.4	300	0	19.07
100	-	2	0	731.1	300	0	19.03
100	-	2	0	701.4	300	0	19.03
100	-	2	0	732.8	300	0	18.98
100	-	2	0	699.8	300	0	18.97
100	-	2	0	734.5	300	0	18.93
100	_	2	0	698.2	300	0	18.91

100	-	2	0	736.2	300	0	18.88
100	_	2	0	696.6	300	0	18.85
100	-	2	0	737.8	300	0	18.82
100	-	2	0	695	300	0	18.78
100	_	2	0	739.5	300	0	18.76
100	-	2	0	693.4	300	0	18.7
100	-	2	0	741.3	300	0	18.69
100	-	2	0	1000	300	0	18.65
100	-	2	0	997.7	300	0	18.63
100	-	2	0	743	300	0	18.63
100	-	2	0	691.8	300	0	18.62
100	-	2	0	995.4	300	0	18.6
100	-	2	0	744.7	300	0	18.56
100	-	2	0	993.1	300	0	18.55
100	_	2	0	690.2	300	0	18.53
100	-	2	0	746.4	300	0	18.49
100	_	2	0	990.8	300	0	18.48
100	_	2	0	688.6	300	0	18.44
100	_	2	0	748.1	300	0	18.41
100	-	2	0	988.6	300	0	18.41
100	-	2	0	687	300	0	18.34
100	-	2	0	749.8	300	0	18.34
100	-	2	0	986.3	300	0	18.31
100	-	2	0	751.6	300	0	18.26
100	-	2	0	685.4	300	0	18.24
100	-	2	0	984	300	0	18.21
100	-	2	0	753.3	300	0	18.18
100	-	2	0	683.8	300	0	18.14
100	-	2	0	755	300	0	18.1
100	-	2	0	981.7	300	0	18.09
100	-	2	0	682.3	300	0	18.03
100	-	2	0	756.8	300	0	18.01
100	-	2	0	979.5	300	0	17.97

The highest attenuation of 18.8 dB/km is achieved with a particle radius of about 716 μ m, and attenuation above 18.0 dB/km occurs for a particle radius in the range of 682 to 757 μ m. However, such large particles settle rapidly. Using a material with ultra-high permittivity (e.g. CaCu3Ti4O12 with a value of 105 in the microwave region and a corresponding refractive index of 10.2 – Yang, 2017), the optimal particle radius can be reduced to 140 μ m (= 716 * 2.0/10.2).

Appendix 2.3. Particle surface potential optimization

Attenuation can also be increased by resonant absorption due to the presence of an electric charge on the particle surface. Typical desert dust particles with the parameters cited in (Kandler, 2009), in the air with a relative humidity of 40%, were used in the computations. The refractive index of wet particles was obtained with our tool "eps2n.exe" (see instructions for the program "visibility.exe"). The optimal value of the potential from the interval 0 to 100 V and the radius of the particles from the interval 0.1 to 1 μ m were searched. Note that the parameters REFR_INDEX_REAL and REFR_INDEX_IMAG are ignored in our case (MATERIALS 2). We store 5,000 of the most advantageous combinations of radius and potential, the total number of tested combinations is about 100,000.

Input parameters for "attenuation.exe":

```
maroko_burka_n.dat
mediterian_n.dat
REFR_INDEX_REAL 0 0 1 LIN
REFR_INDEX_IMAG 0 0 1 LIN
RADIUS 1e-1 1e0 500 LIN
TEMPERATURE 300 300 1 LIN
POTENTIAL 0 100 101 LIN
COEFF 1
SHOW_BEST 5000
```

First lines of the file "attenuation.dat":

f[GHz]	material	real(n) imag(n) r[mkm]	tem.[K] pot.[V]	att.[d	lB/km]	
30	maroko_burka_n.dat	2.584	0.03205	7.1683e-001	300	92	1.422
30	maroko_burka_n.dat	2.584	0.03205	7.4749e-001	300	100	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.9699e-001	300	87	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.8076e-001	300	83	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.4289e-001	300	74	1.422
30	maroko_burka_n.dat	2.584	0.03205	7.2044e-001	300	93	1.422
30	maroko_burka_n.dat	2.584	0.03205	5.9780e-001	300	64	1.422
30	maroko_burka_n.dat	2.584	0.03205	7.4389e-001	300	99	1.422
30	maroko_burka_n.dat	2.584	0.03205	5.4910e-001	300	54	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.5551e-001	300	77	1.422
30	maroko_burka_n.dat	2.584	0.03205	7.1323e-001	300	91	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.6814e-001	300	80	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.3387e-001	300	72	1.422
30	maroko_burka_n.dat	2.584	0.03205	6.6453e-001	300	79	1.422

The highest achievable attenuation at a given particle concentration is about 1.4 dB/km for quartz dust ("maroko_burka_n.dat"). We processed the file "attenuation.dat" in MS EXCEL and displayed the points with the highest attenuation as a dependence of radius (Figure 4):

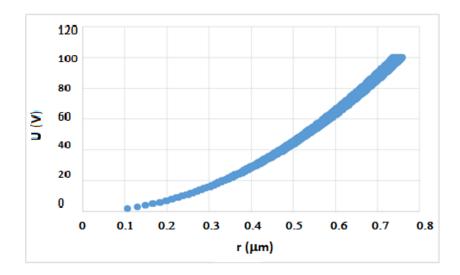


Fig. 4. Dependence of the optimal potential value on the particle radius for SiO₂

The graph in Figure 4 is analogous to Figure 1 from the article (Kocifaj, 2015).

References

Kandler, 2009 K. Kandler et al: Size distribution, mass concentration, chemical and mineralogical composition and derived optical parameters of the boundary layer aerosol at Tinfou, Morocco, during SAMUM 2006. Tellus (2009), 61B, 32-50. Kocifaj, 2015 Miroslav Kocifaj, Jozef Klačka, František Kundracik and Gorden Videen: Chargeinduced electromagnetic resonances in nanoparticles. Ann. Phys. (Berlin) 527, No. 11-12, 765-769 (2015) Kocifaj, 2016 Miroslav Kocifaj, František Kundracik, Gorden Videen: Optical characterization of electrically charged particles using discrete dipole approximation. Journal of Quantitative Spectroscopy & Radiative Transfer 184 (2016) 161–166 Yang, 2017 C. P. Yang, X. Y. Luo, D. W. Shi, H. B. Xiao, L. F. Xu and K. Barner: he dielectric constant of CaCu3Ti4O12 ceramics. J Material Sci Eng 2017, 6:4(Suppl) DOI: 10.4172/2169-0022-C1-071