Sensitivity of Aerosol Refractive Indices and Impact on CRTM Scattering Calculations

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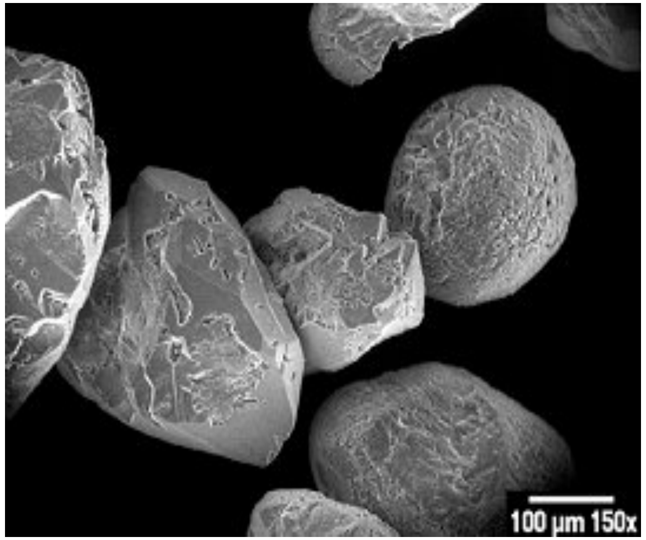
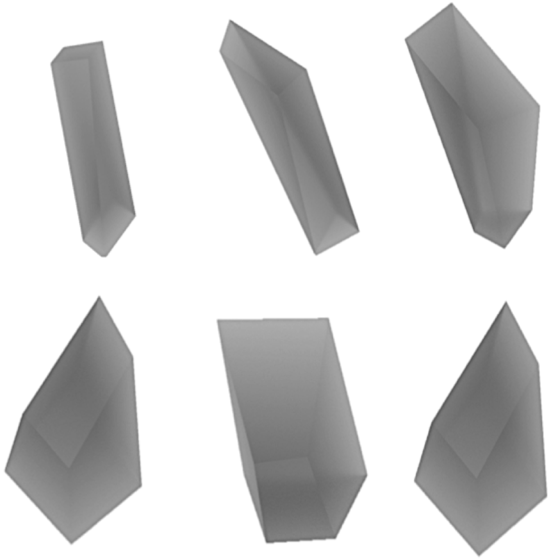
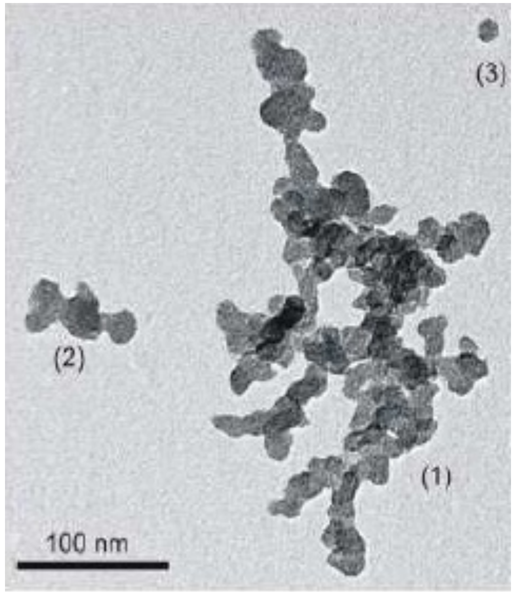
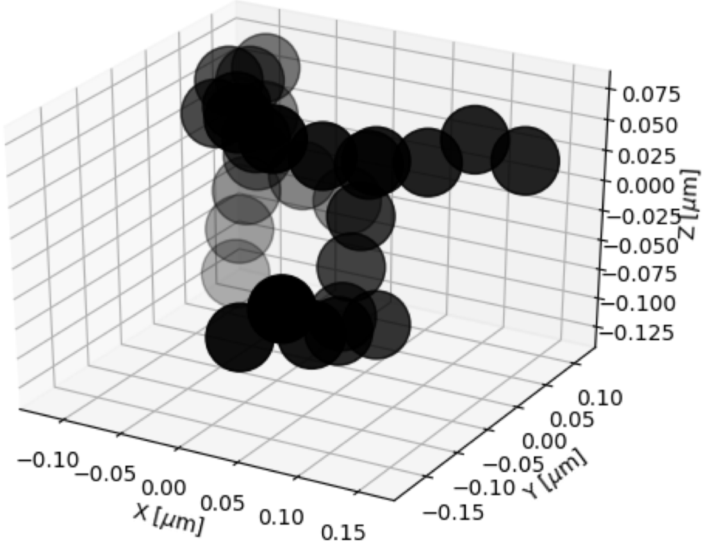
Light scattering by aerosols









Light scattering calculations for aerosols require assumptions about:

- Particle shape
- Particle number size distribution
- **<u>Refractive index</u>**

Literature research for existing refractive index spectra

Table 8. Montmorillonite Pellet. PAGE 5

WN	WL	N	K	DN	DK	R
2050.00	4.8780	1.391	0.034	0.010	0.011	0.02740
2060.00	4.8544	1.391	0.033	0.010	0.011	0.02745
2070.00	4.8309	1.393	0.032	0.010	0.011	0.02760
2080.00	4.8077	1.394	0.033	0.010	0.011	0.02780
2090.00	4.7847	1.394	0.032	0.010	0.011	0.02775
2100.00	4.7619	1.397	0.031	0.010	0.011	0.02810
2110.00	4.7393	1.399	0.032	0.010	0.011	0.02830
2120.00	4.7170	1.399	0.033	0.010	0.011	0.02835
2130.00	4.6948	1.398	0.033	0.010	0.011	0.02825
2140.00	4.6729	1.400	0.031	0.010	0.011	0.02840
2150.00	4.6512	1.402	0.032	0.010	0.011	0.02875
2160.00	4.6296	1.404	0.033	0.010	0.011	0.02895
2170.00	4.6083	1.403	0.036	0.010	0.011	0.02890
2180.00	4.5872	1.402	0.034	0.010	0.011	0.02870
2190.00	4.5662	1.404	0.033	0.010	0.011	0.02900
2200.00	4.5455	1.404	0.035	0.010	0.011	0.02895
2210.00	4.5249	1.403	0.033	0.010	0.011	0.02880
2220.00	4.5045	1.404	0.032	0.010	0.011	0.02900
2230.00	4.4843	1.405	0.031	0.009	0.011	0.02905
2240.00	4.4643	1.409	0.031	0.009	0.012	0.02950
2250.00	4.4444	1.408	0.035	0.010	0.012	0.02945
2260.00	4.4248	1.406	0.032	0.009	0.011	0.02920
2270.00	4.4053	1.409	0.031	0.009	0.012	0.02955
2280.00	4.3860	1.410	0.033	0.009	0.012	0.02965
2290.00	4.3668	1.409	0.033	0.009	0.012	0.02955
2300.00	4.3478	1.409	0.031	0.009	0.012	0.02950
2310.00	4.3290	1.412	0.031	0.009	0.012	0.02985
2320.00	4.3103	1.411	0.031	0.009	0.012	0.02975
2330.00	4.2918	1.413	0.030	0.009	0.012	0.03000
2340.00	4.2735	1.415	0.031	0.009	0.012	0.03025
2350.00	4.2553	1.415	0.033	0.009	0.012	0.03030
2360.00	4.2373	1.414	0.032	0.009	0.012	0.03015
2370.00	4.2194	1.416	0.032	0.009	0.012	0.03040
2380.00	4.2017	1.415	0.033	0.009	0.012	0.03030
2390.00	4.1841	1.416	0.033	0.009	0.012	0.03040
2400.00	4.1667	1.414	0.032	0.009	0.012	0.03010
2410.00	4.1494	1.417	0.028	0.009	0.012	0.03040
2420.00	4.1322	1.421	0.031	0.009	0.012	0.03095
2430.00	4.1152	1.419	0.034	0.009	0.012	0.03070
2440.00	4.0984	1.418	0.032	0.009	0.012	0.03060
2450.00	4.0816	1.421	0.031	0.009	0.012	0.03090
2460.00	4.0650	1.422	0.033	0.009	0.012	0.03110
2470.00	4.0486	1.420	0.034	0.009	0.012	0.03085
2480.00	4.0323	1.421	0.033	0.009	0.012	0.03095
2490.00	4.0161	1.421	0.034	0.009	0.012	0.03095
2500.00	4.0000	1.422	0.033	0.009	0.012	0.03105
2510.00	3.9841	1.421	0.033	0.009	0.012	0.03100
2520.00	3.9683	1.422	0.034	0.009	0.012	0.03115
2530.00	3.9526	1.421	0.034	0.009	0.012	0.03095
2540.00	3.9370	1.422	0.032	0.009	0.012	0.03110

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Table 8. Montmorillonite Pellet. PAGE 3

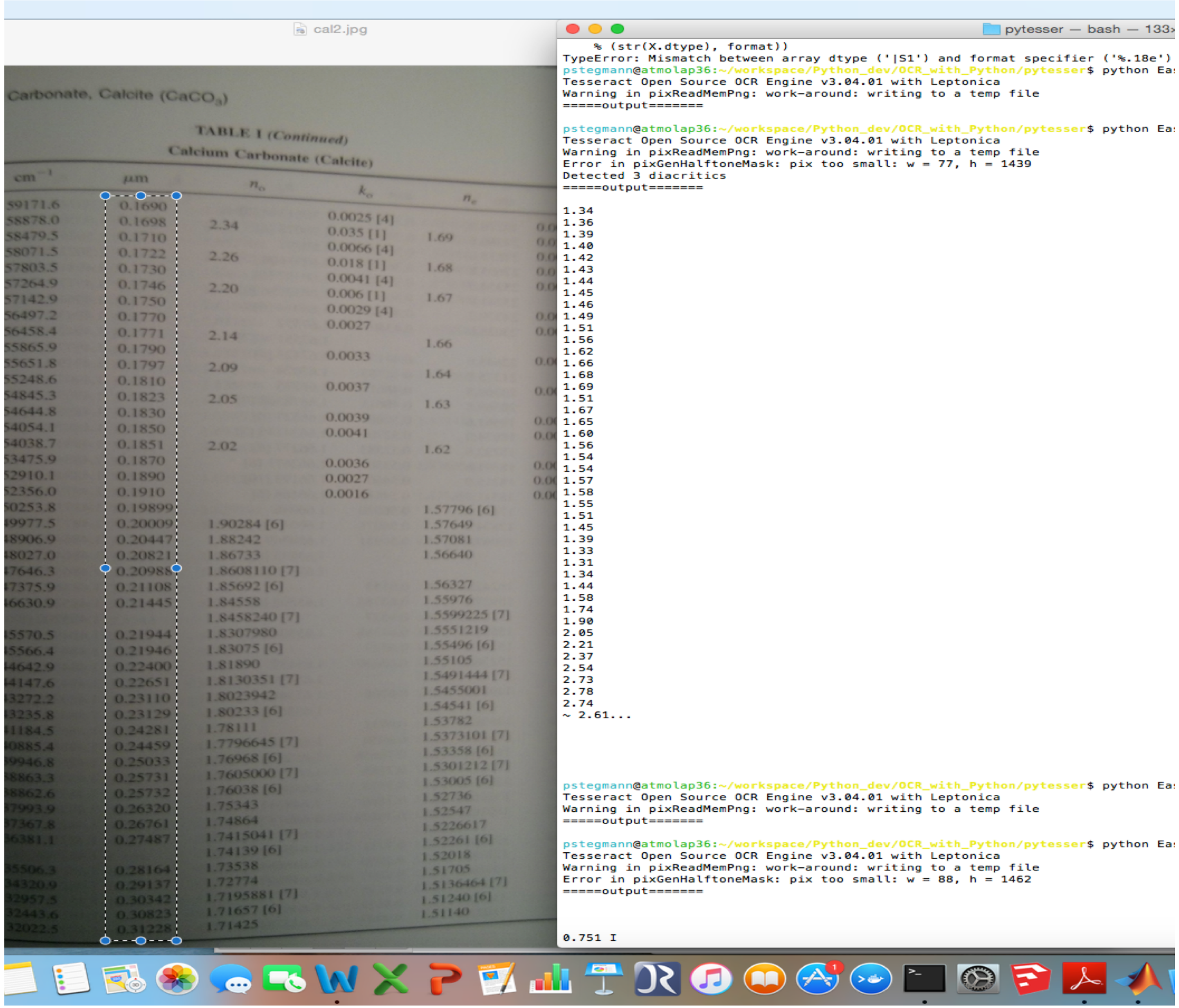
WN	WL	N	K	DN	DK	R
1050.00	9.5238	1.828	1.892	0.077	0.018	0.37090
1060.00	9.4340	1.33				
1070.00	9.3458	0.89				
1080.00	9.2593	0.70				
1090.00	9.1743	0.71				
1100.00	9.0909	0.79				
1110.00	9.0090	0.88				
1120.00	8.9286	0.89				
1130.00	8.8496	0.79				
1140.00	8.7719	0.71				
1150.00	8.6957	0.67				
1160.00	8.6207	0.67				
1170.00	8.5470	0.70				
1180.00	8.4746	0.72				
1190.00	8.4034	0.77				
1200.00	8.3333	0.83				
1210.00	8.2645	0.88				
1220.00	8.1967	0.92				
1230.00	8.1301	0.96				
1240.00	8.0645	1.00				
1250.00	8.0000	1.03				
1260.00	7.9365	1.05				
1270.00	7.8740	1.08				
1280.00	7.8125	1.10				
1290.00	7.7519	1.11				
1300.00	7.6923	1.12				
1310.00	7.6336	1.13				
1320.00	7.5758	1.15				
1330.00	7.5188	1.17				
1340.00	7.4627	1.18				
1350.00	7.4074	1.19				
1360.00	7.3529	1.21				
1370.00	7.2993	1.22				
1380.00	7.2464	1.22				
1390.00	7.1942	1.23				
1400.00	7.1429	1.24				
1410.00	7.0922	1.24				
1420.00	7.0423	1.25				
1430.00	6.9930	1.25				
1440.00	6.9444	1.26				
1450.00	6.8966	1.26				
1460.00	6.8493	1.26				
1470.00	6.8027	1.26				
1480.00	6.7568	1.27				
1490.00	6.7114	1.28				
1500.00	6.6667	1.28				
1510.00	6.6225	1.28				
1520.00	6.5789	1.29				
1530.00	6.5359	1.29				
1540.00	6.4935	1.29				

Table 8. Montmorillonite Pellet. PAGE 4

WN	WL	N	K	DN	DK	R
1550.00	6.4516	1.304	0.051	0.011	0.009	0.01820
1560.00	6.4103	1.307	0.051	0.011	0.010	0.01860
1570.00	6.3694	1.313	0.048	0.011	0.010	0.01910
1580.00	6.3291	1.318	0.050	0.011	0.010	0.01970
1590.00	6.2893	1.321	0.050	0.011	0.010	0.02000
1600.00	6.2500	1.325	0.051	0.011	0.010	0.02040
1610.00	6.2112	1.329	0.050	0.011	0.010	0.02085
1620.00	6.1728	1.331	0.054	0.011	0.010	0.02105
1630.00	6.1350	1.330	0.051	0.011	0.010	0.02095
1640.00	6.0976	1.335	0.050	0.011	0.010	0.02140
1650.00	6.0606	1.337	0.049	0.011	0.010	0.02165
1660.00	6.0241	1.341	0.048	0.011	0.010	0.02210
1670.00	5.9880	1.346	0.048	0.011	0.010	0.02265
1680.00	5.9524	1.353	0.053	0.011	0.011	0.02350
1690.00	5.9172	1.352	0.063	0.011	0.011	0.02360
1700.00	5.8824	1.344	0.064	0.011	0.011	0.02270
1710.00	5.8480	1.343	0.061	0.011	0.011	0.02250
1720.00	5.8140	1.340	0.059	0.011	0.010	0.02215
1730.00	5.7803	1.338	0.053	0.011	0.010	0.02185
1740.00	5.7471	1.341	0.048	0.011	0.010	0.02205
1750.00	5.7143	1.345	0.046	0.010	0.010	0.02240
1760.00	5.6818	1.347	0.043	0.010	0.010	0.02260
1770.00	5.6497	1.352	0.041	0.010	0.010	0.02315
1780.00	5.6180	1.355	0.042	0.010	0.010	0.02345
1790.00	5.5866	1.358	0.041	0.010	0.010	0.02375
1800.00	5.5556	1.359	0.043	0.010	0.010	0.02395
1810.00	5.5249	1.361	0.041	0.010	0.010	0.02410
1820.00	5.4945	1.362	0.042	0.010	0.011	0.02430
1830.00	5.4645	1.363	0.040	0.010	0.011	0.02430
1840.00	5.4348	1.367	0.040	0.010	0.011	0.02480
1850.00	5.4054	1.368	0.042	0.010	0.011	0.02490
1860.00	5.3763	1.367	0.041	0.010	0.011	0.02485
1870.00	5.3476	1.370	0.041	0.010	0.011	0.02510
1880.00	5.3191	1.370	0.040	0.010	0.011	0.02515
1890.00	5.2910	1.372	0.040	0.010	0.011	0.02530
1900.00	5.2632	1.372	0.039	0.010	0.011	0.02530
1910.00	5.2356	1.374	0.038	0.010	0.011	0.02555
1920.00	5.2083	1.375	0.038	0.010	0.011	0.02570
1930.00	5.1813	1.376	0.038	0.010	0.011	0.02575
1940.00	5.1546	1.378	0.037	0.010	0.011	0.02595
1950.00	5.1282	1.379	0.038	0.010	0.011	0.02615
1960.00	5.1020	1.379	0.037	0.010	0.011	0.02610

Optical Character Recognition for Automatic Database Acquisition

- Rarely refractive index values are available as Dispersion Relations.
- Vast data tables are preferred by authors.
- Reading the *huge* databases and typing them in *manually* is time-consuming, error-prone and a bad for the eyes of the reader.
- In response, a simple **Optical Character Recognition** (OCR) code has been developed in *Python*
- OCR code fails if text misalignment is too large, e.g. for books, but provides a huge speed-up and considerable increase in reliability in many other cases, e.g. for PDFs.



Dust composition is modeled based on a size-dependent composition

S/A DUST GROUP MODEL

Database overview

DUST PARTICLE SIZE

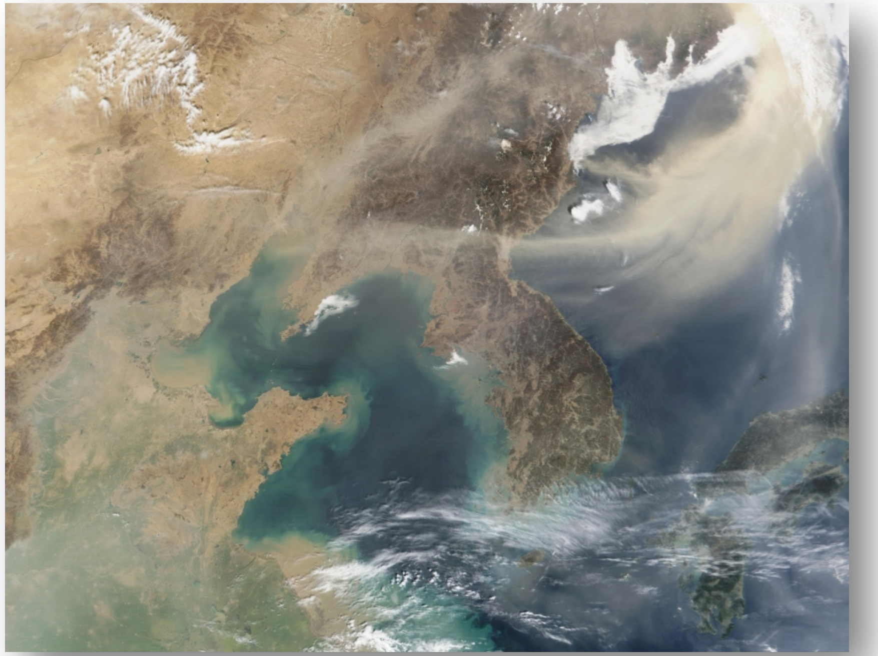
MINERAL REFRACTIVE INDEX SPECTRA

COMPOSITION

BRUGGEMAN MIXING

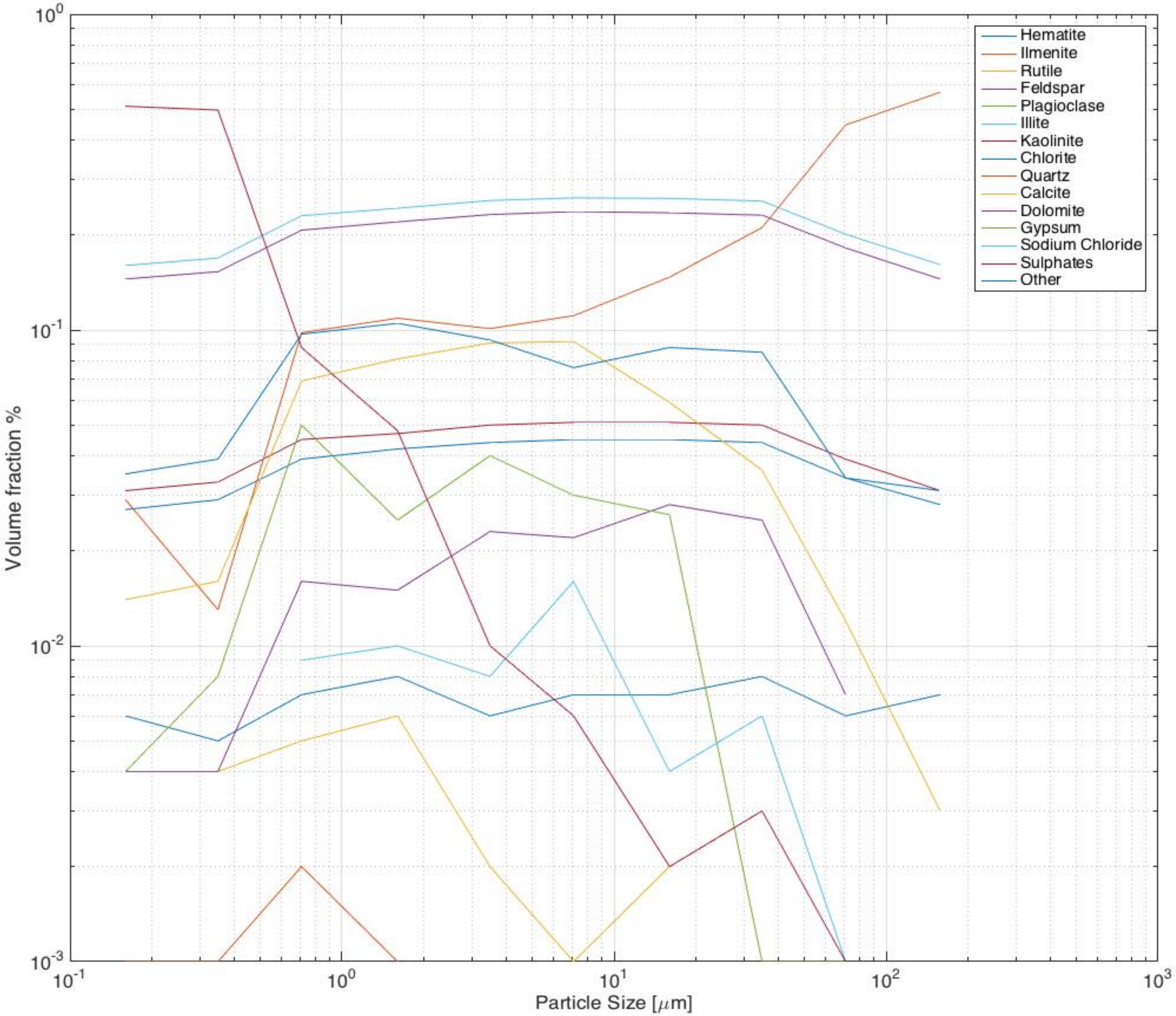
GEOGRAPHIC LOCATION

African or Asian dust



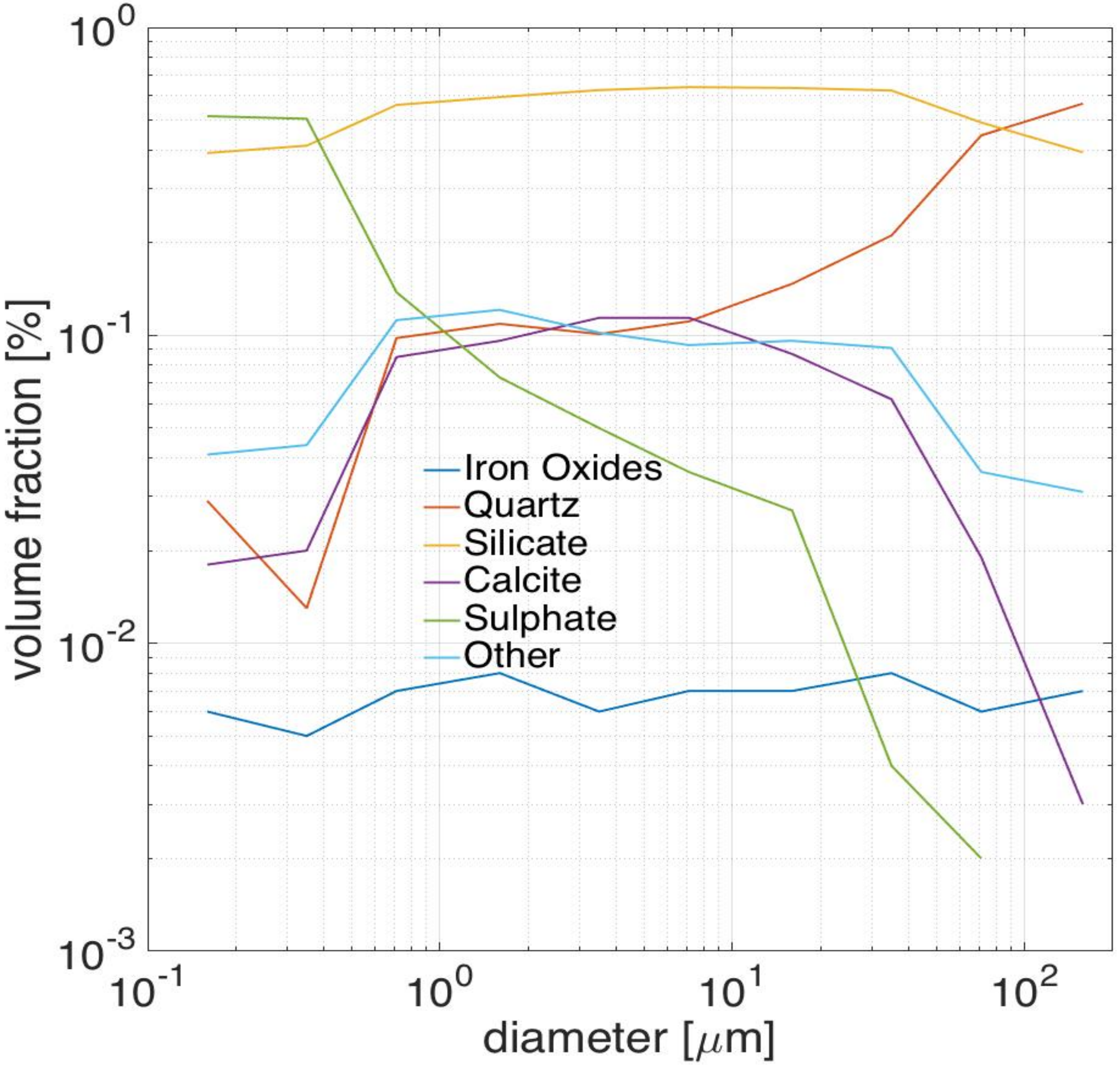
KRAMERS-KRONIG INTEGRAL

Example: Northern Saharan Sand Composition



Actual Composition

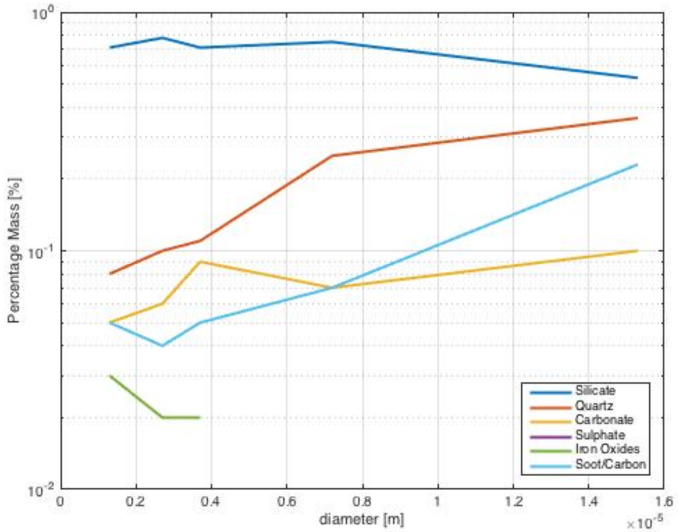
Example: Northern Saharan Sand Composition



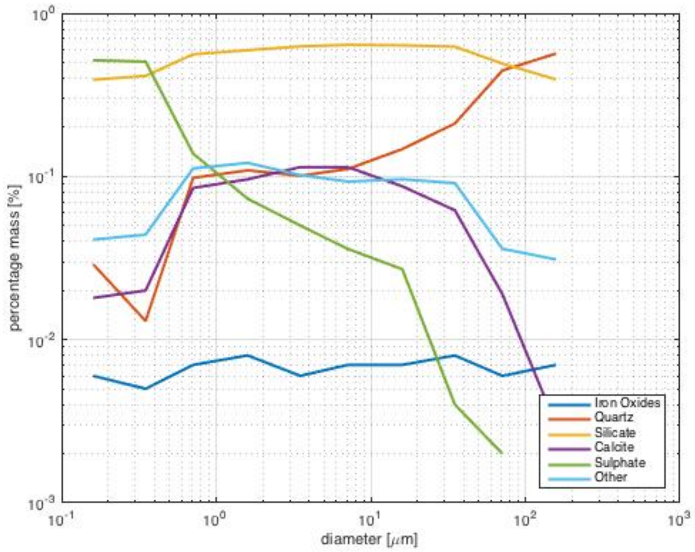
Simplified group model

Regional Dust Composition Overview

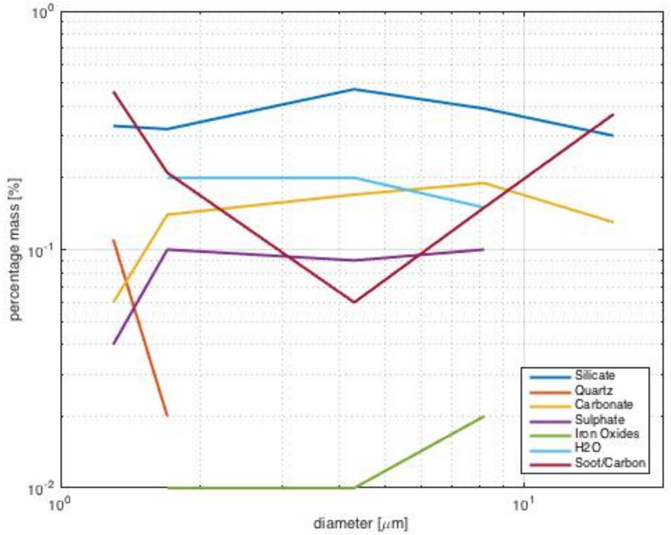
Saharan & Asian Dust composition is decomposed into a number of component groups clustering distinct minerals and chemical species.



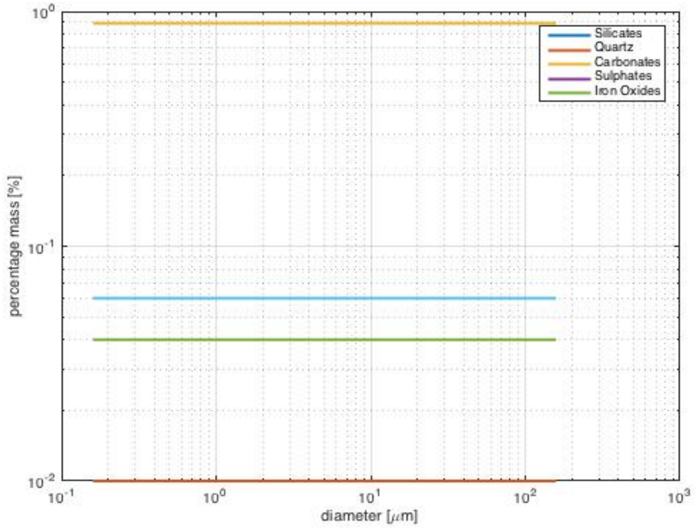
West Asia



Northern Sahara



East Asia



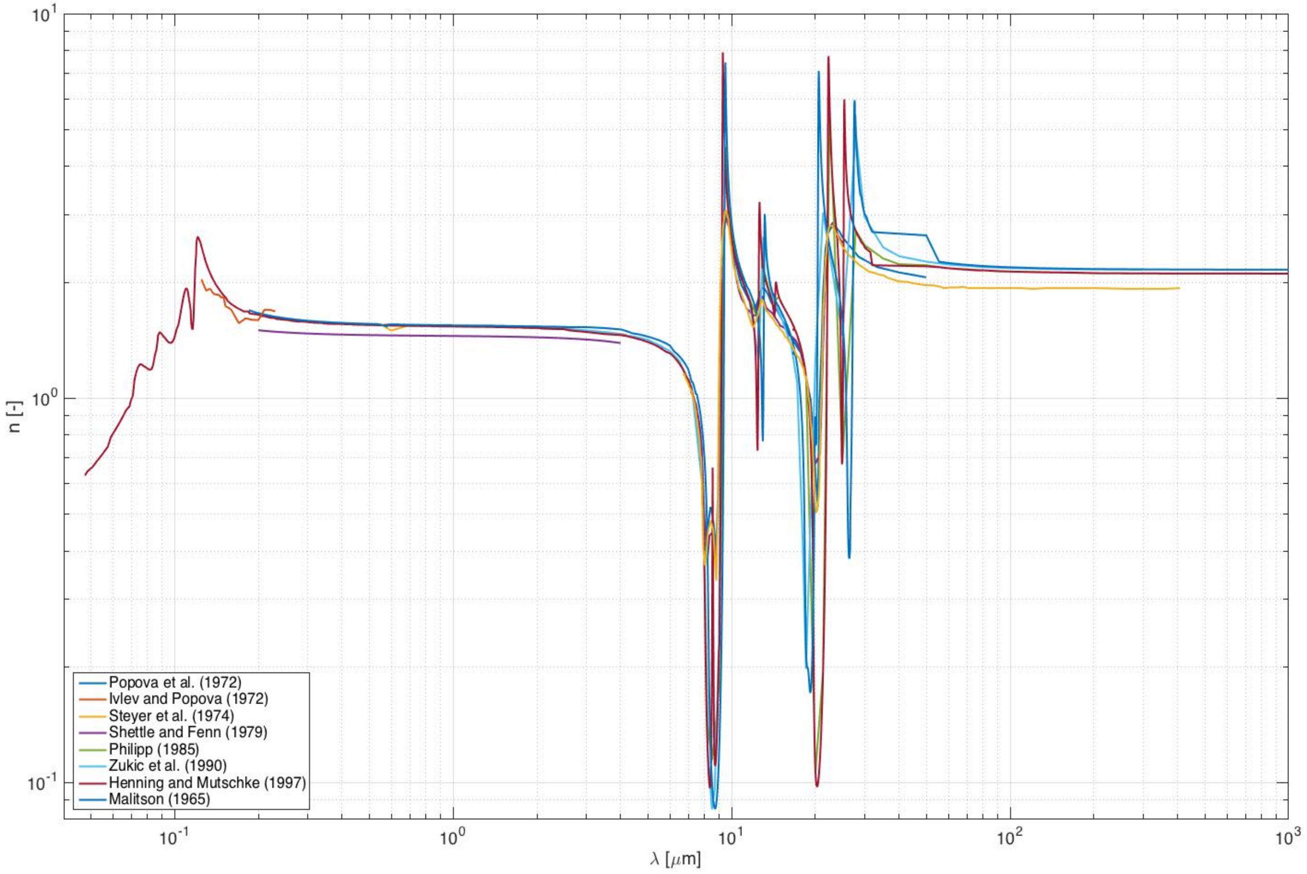
Southern Sahara

Data base acquisition status

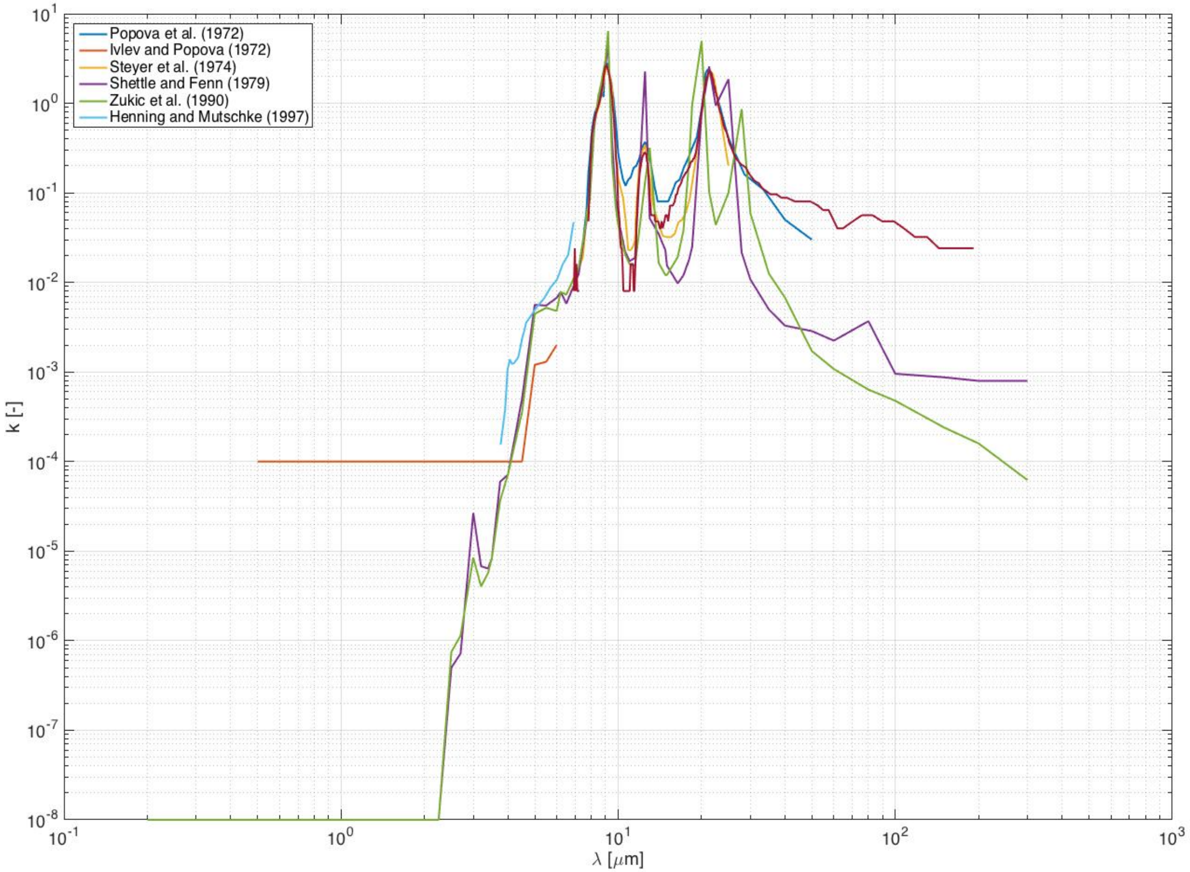
REFRACTIVE INDEX SPECTRA OF INDIVIDUAL MINERALS

Quartz group

All databases for real part.

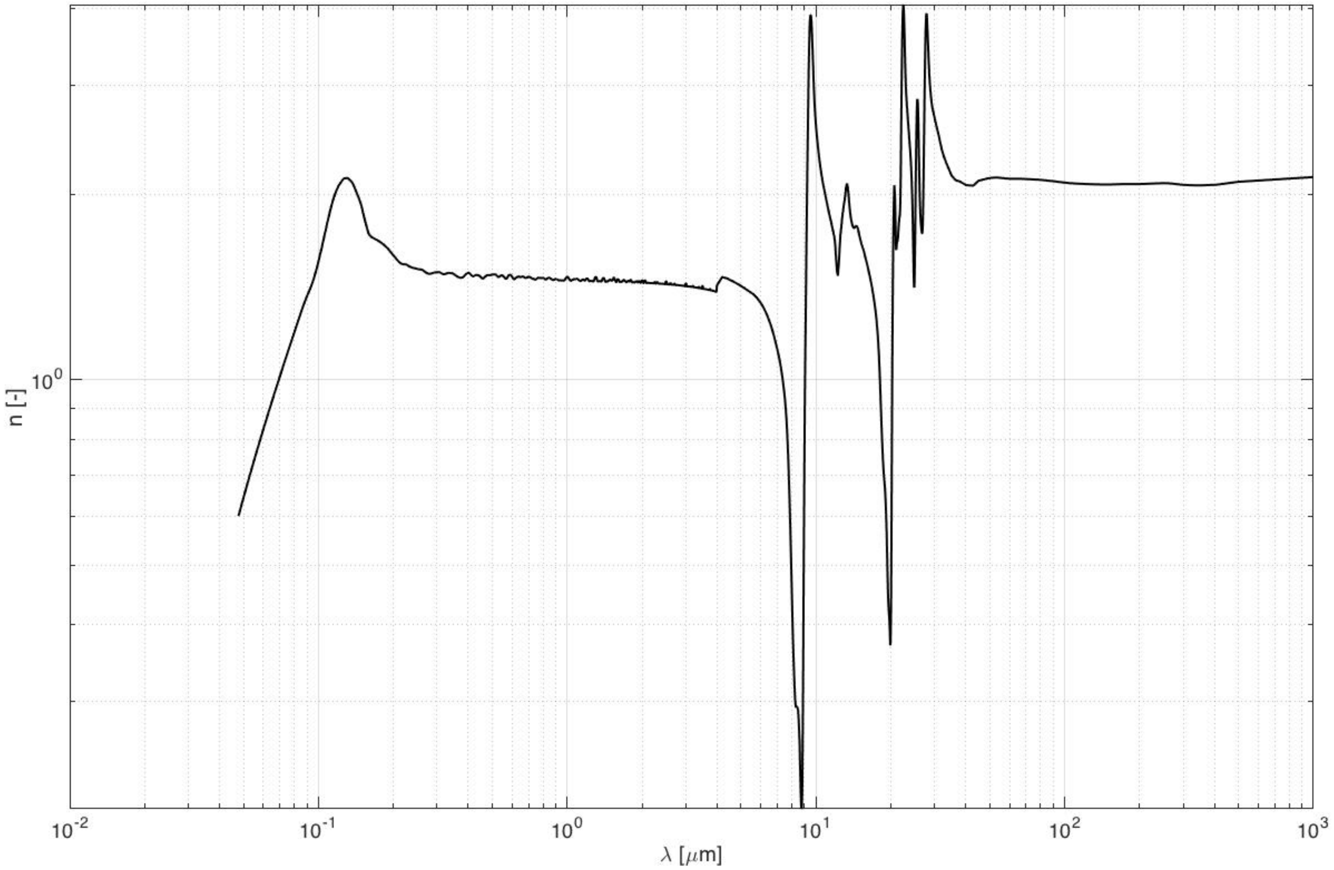


Imaginary part.

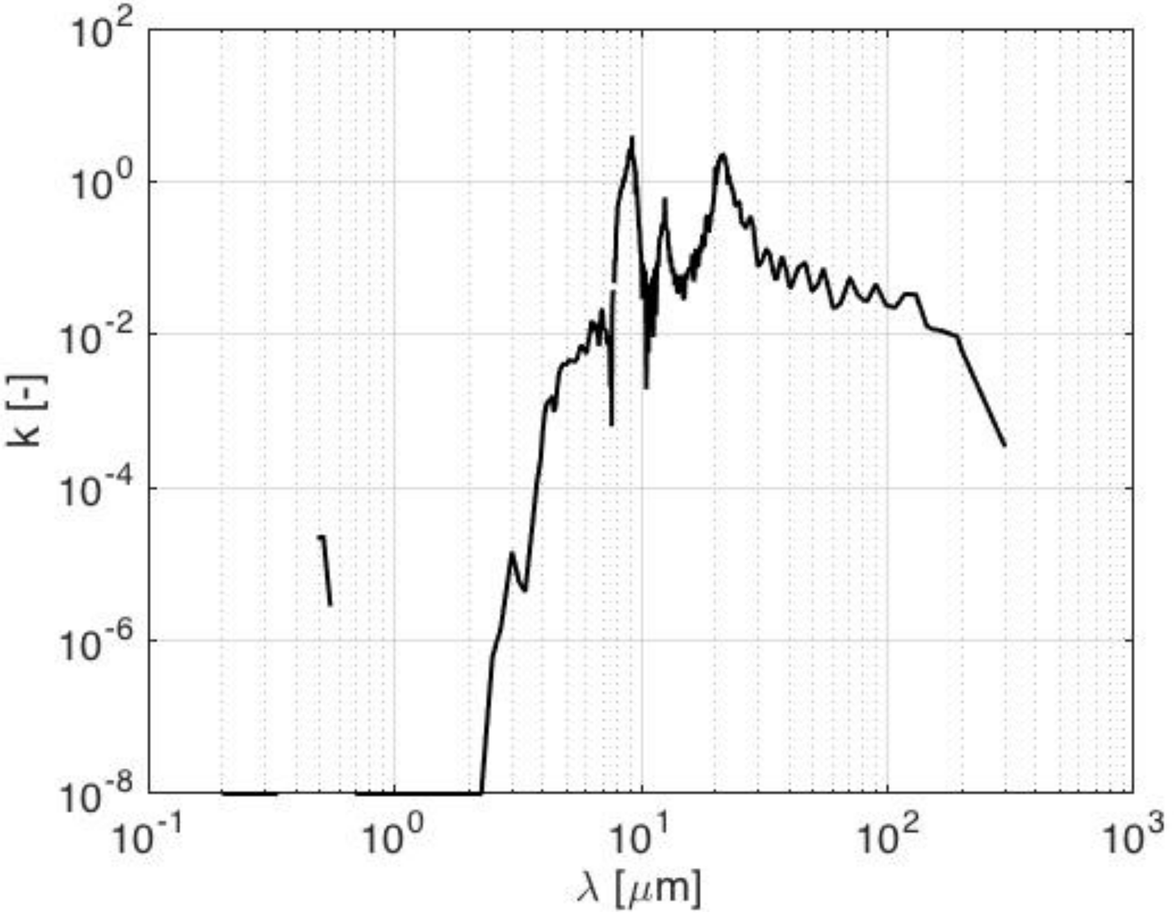


Quartz group (moving average filter)

All databases for real part.

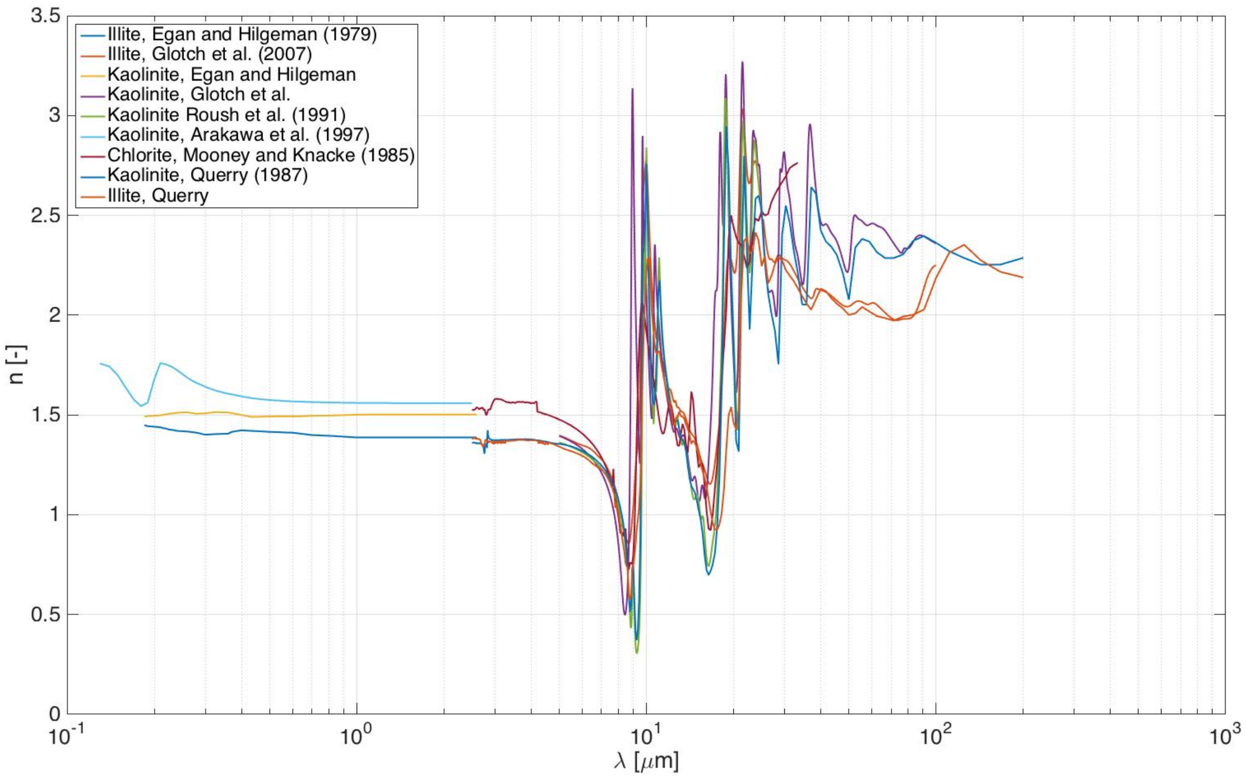


Imaginary part.

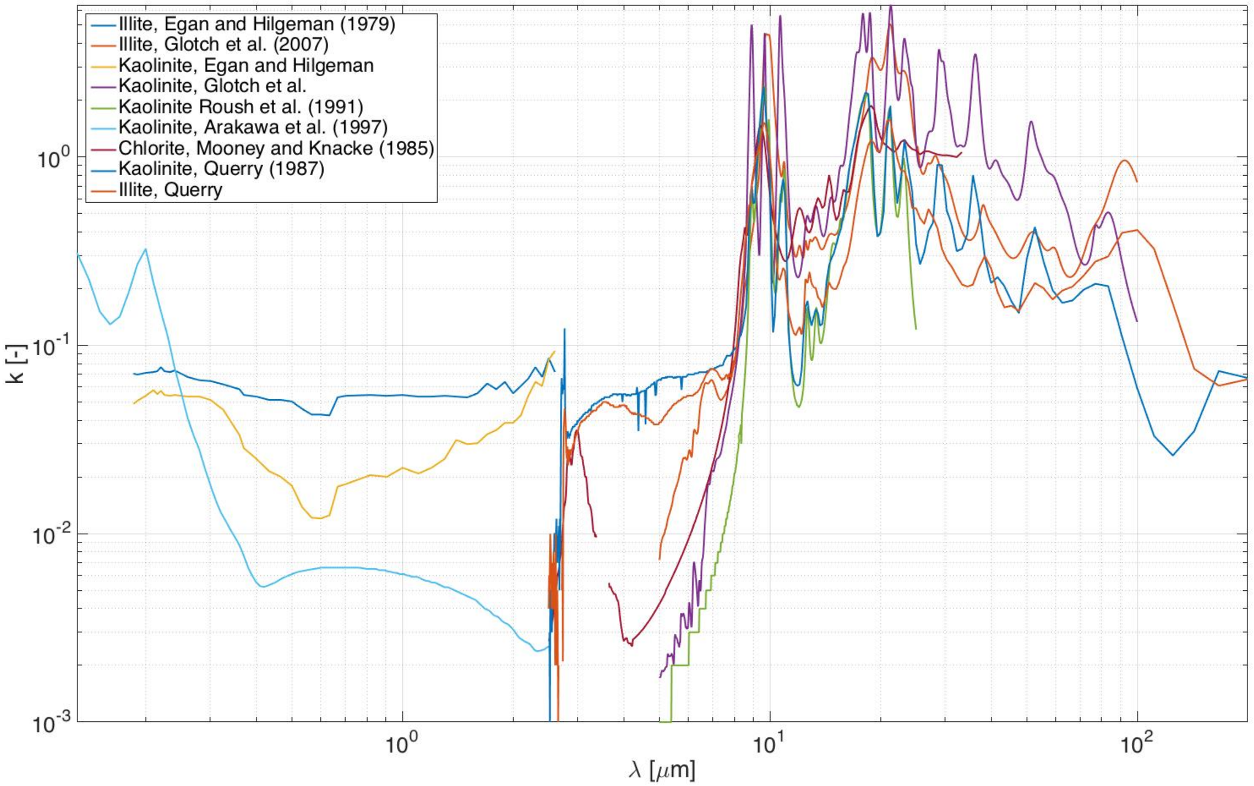


Silicates group

All databases for real part.

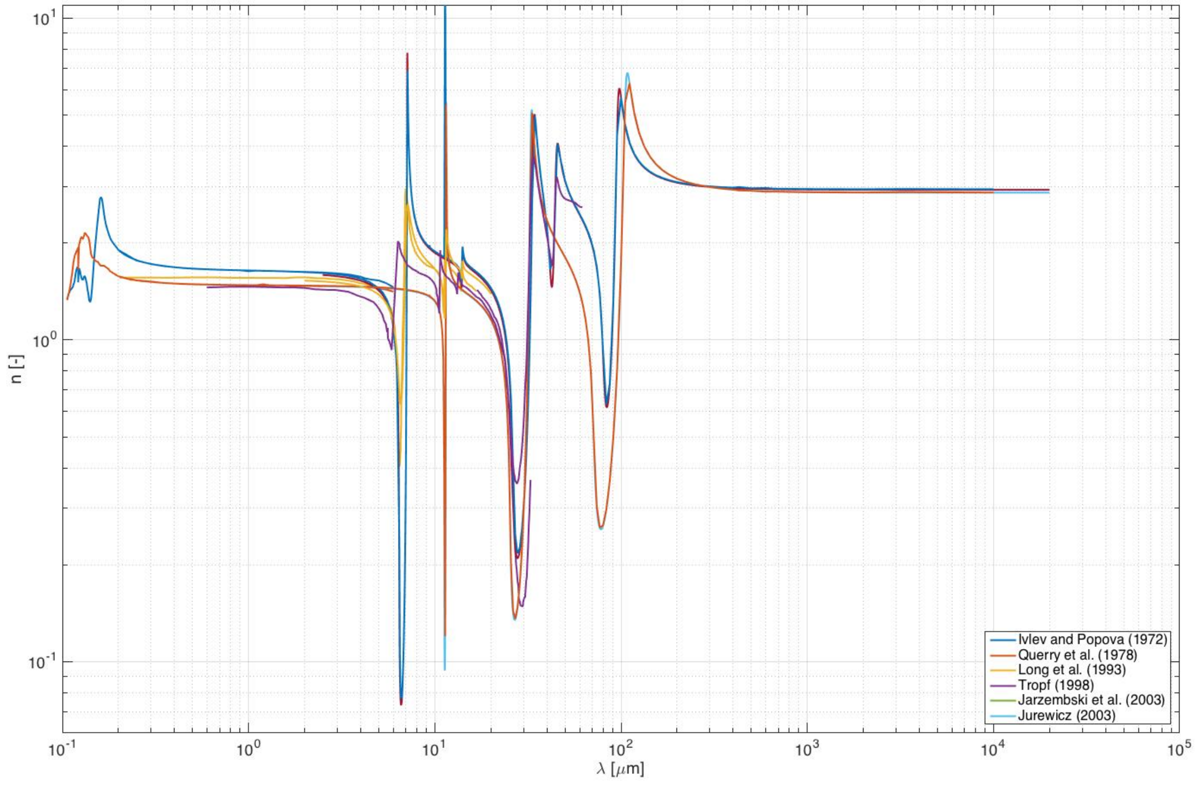


Imaginary part.

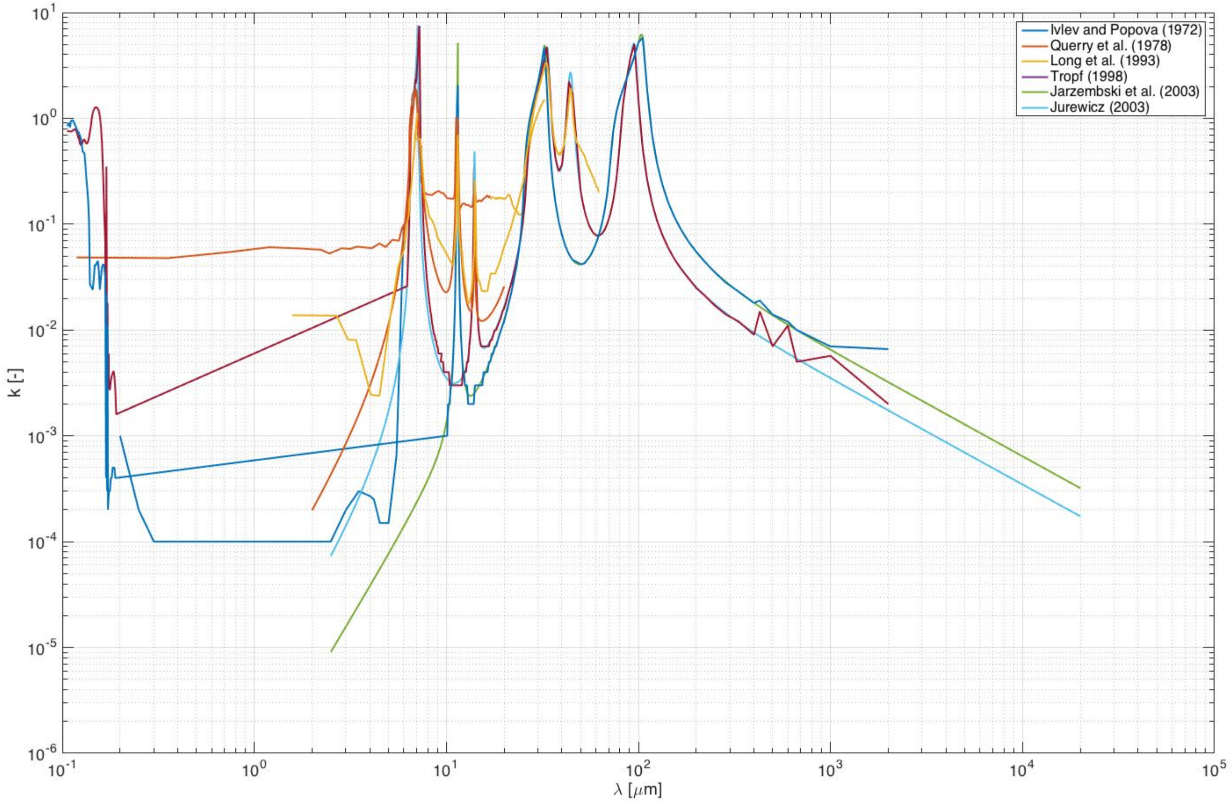


Carbonates group

All databases for real part.

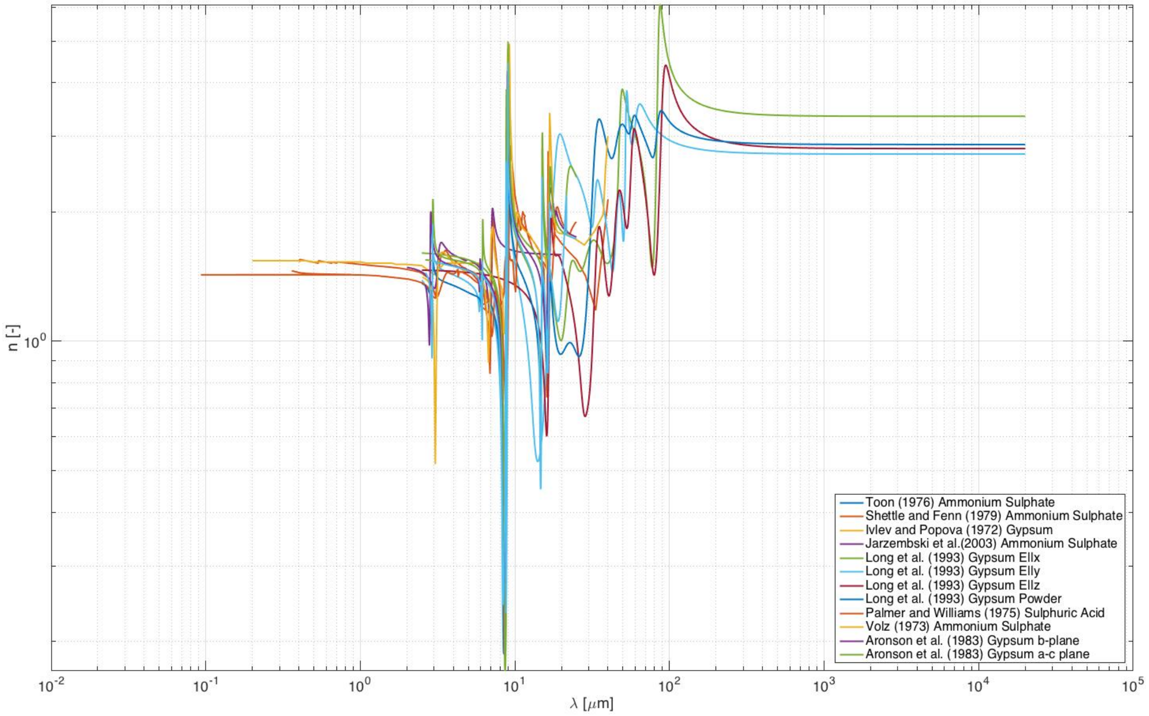


Imaginary part

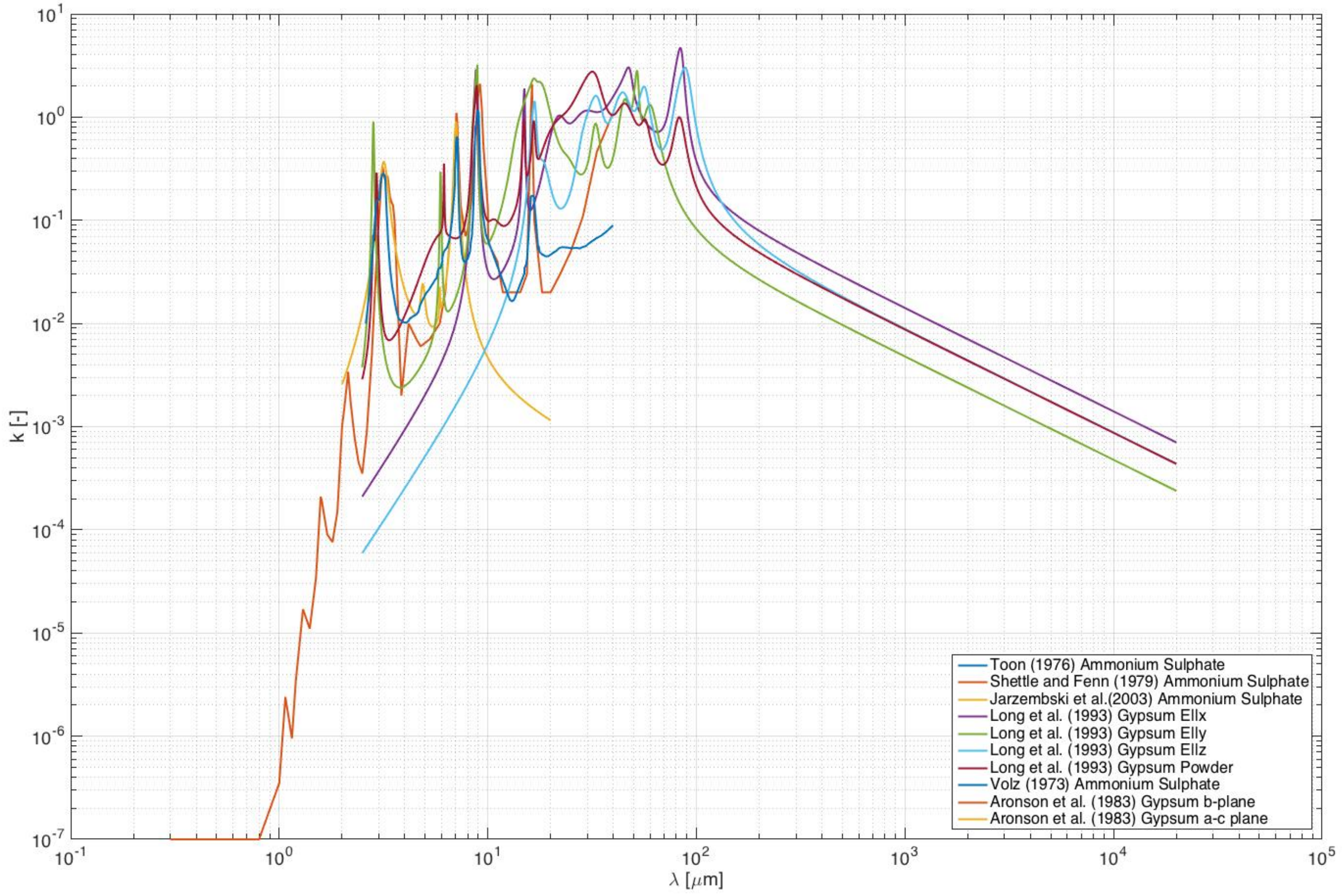


Sulphates group

All databases for real part.

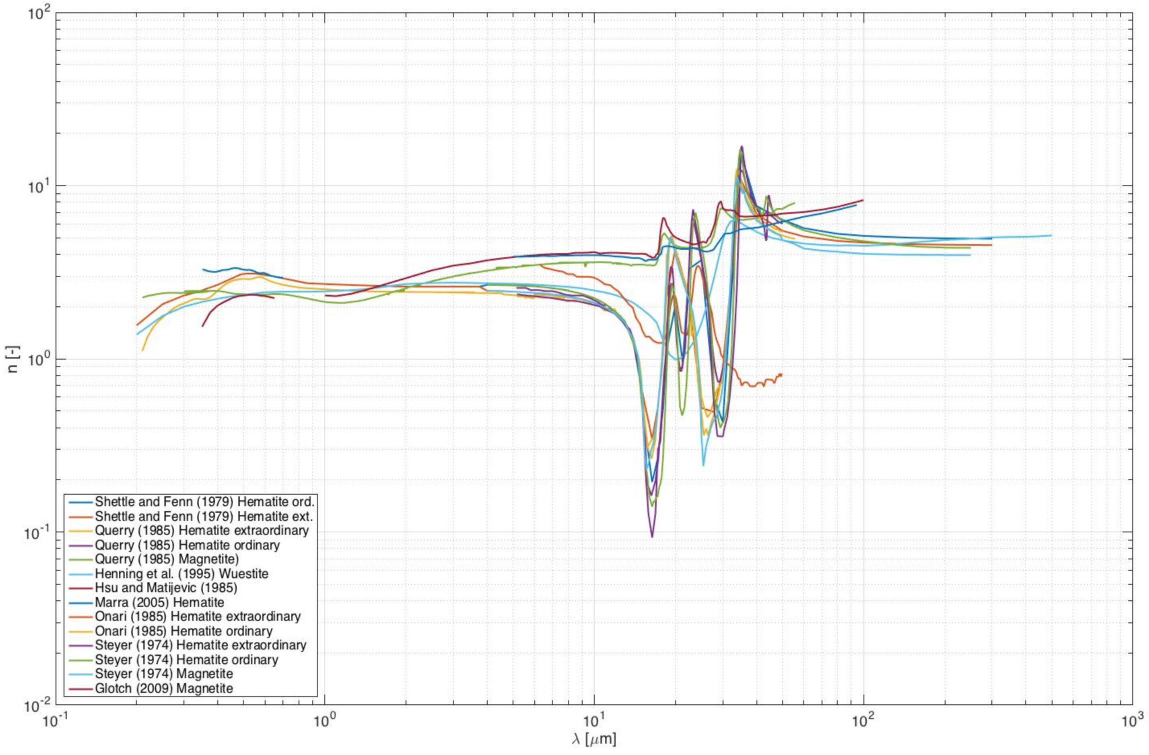


Imaginary part.

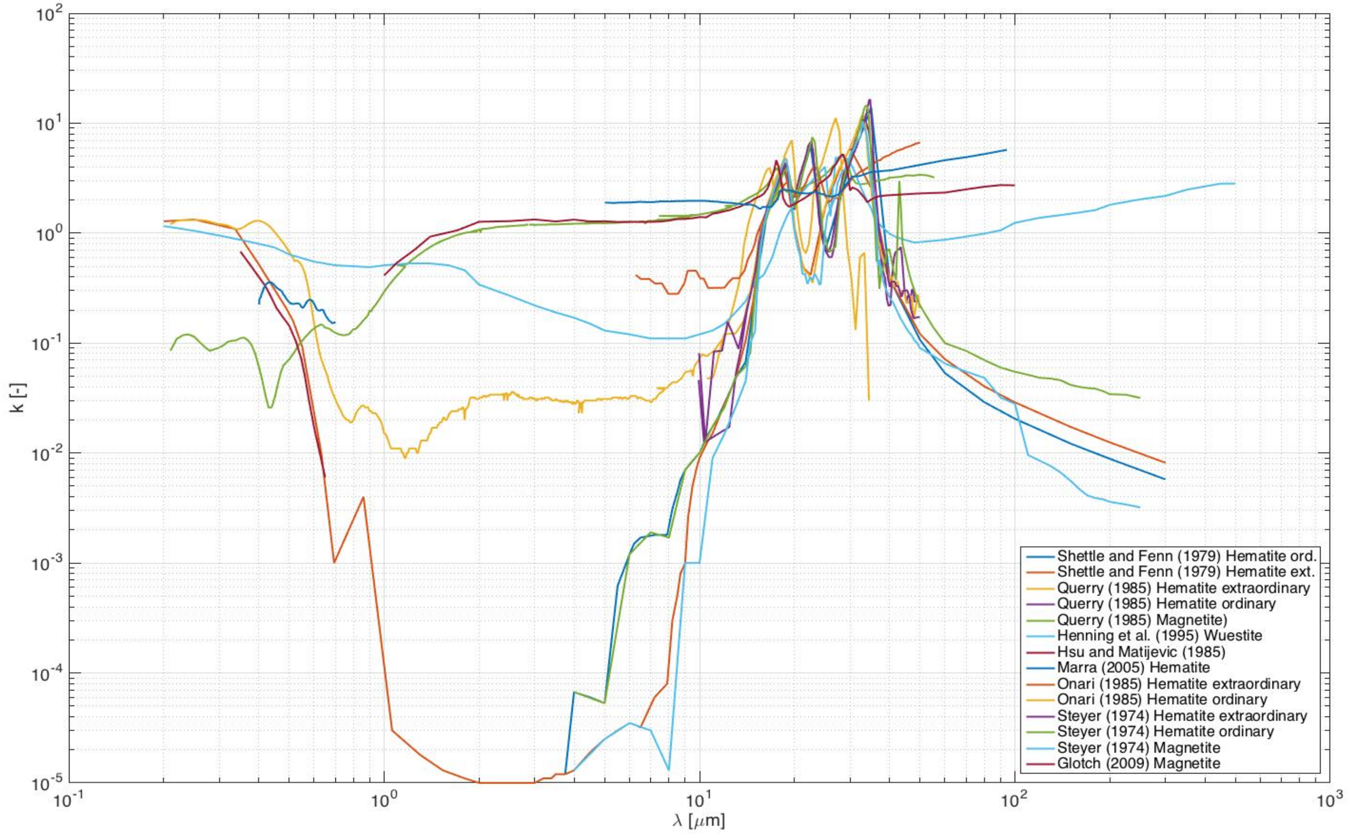


Iron oxides group

All databases for real part.

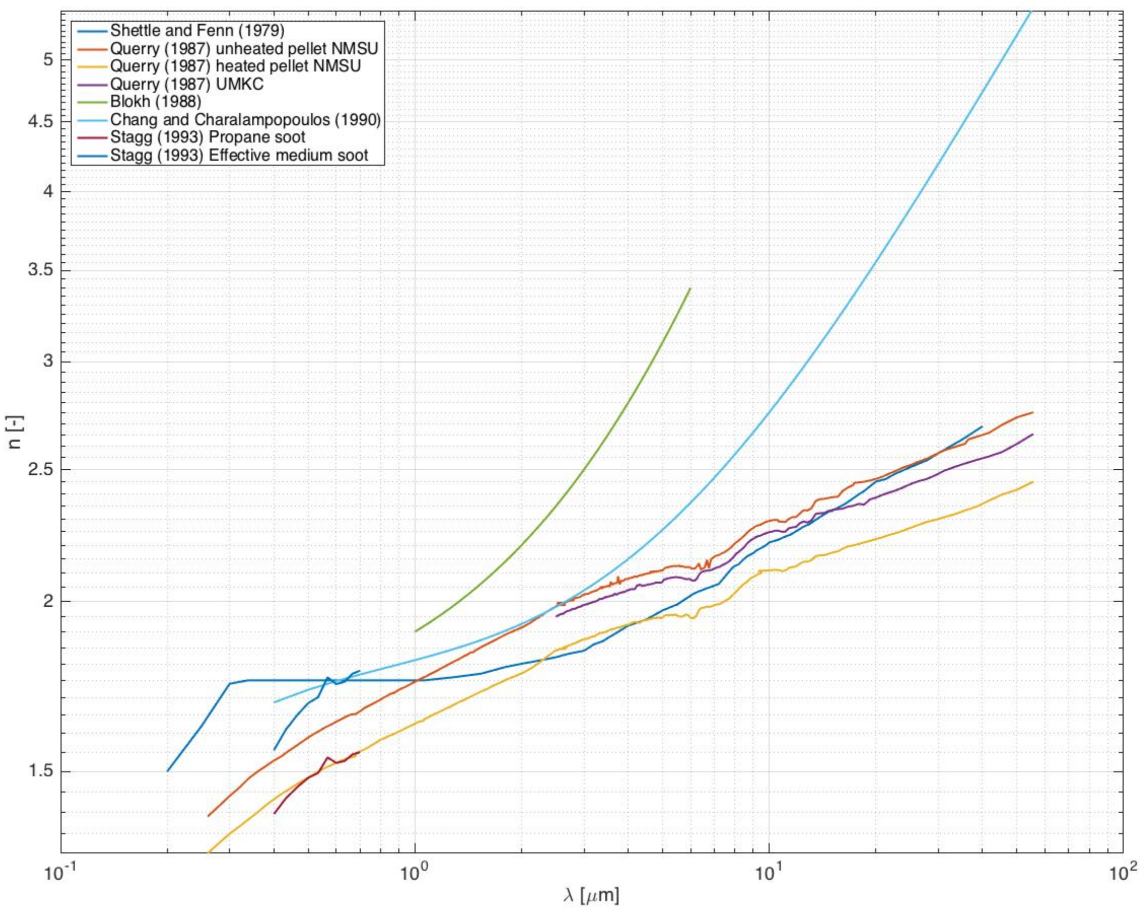


Imaginary part.

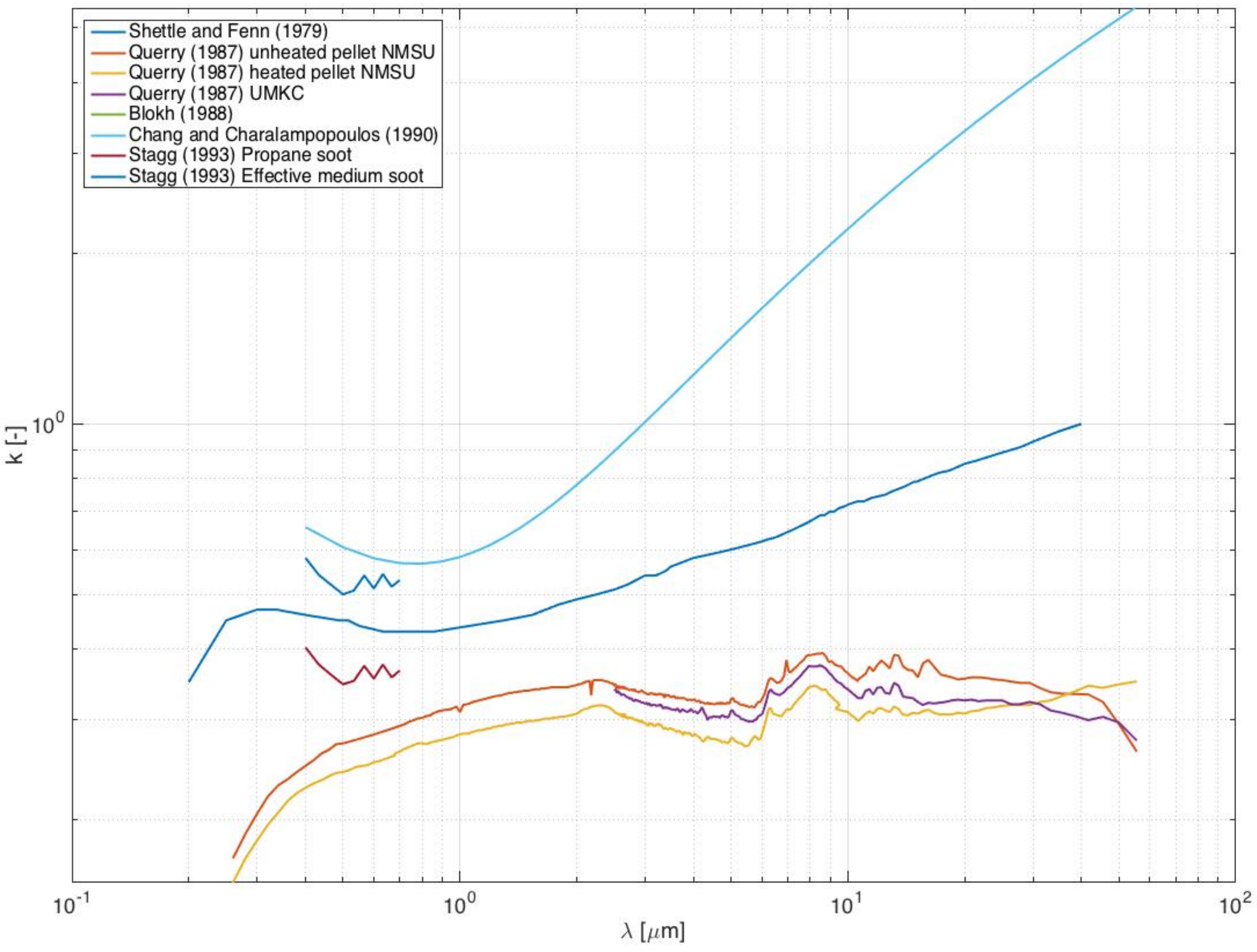


Soot group

All databases for real part



Imaginary Part



Heterogeneous Material

BRUGGEMAN EFFECTIVE MEDIUM APPROXIMATION

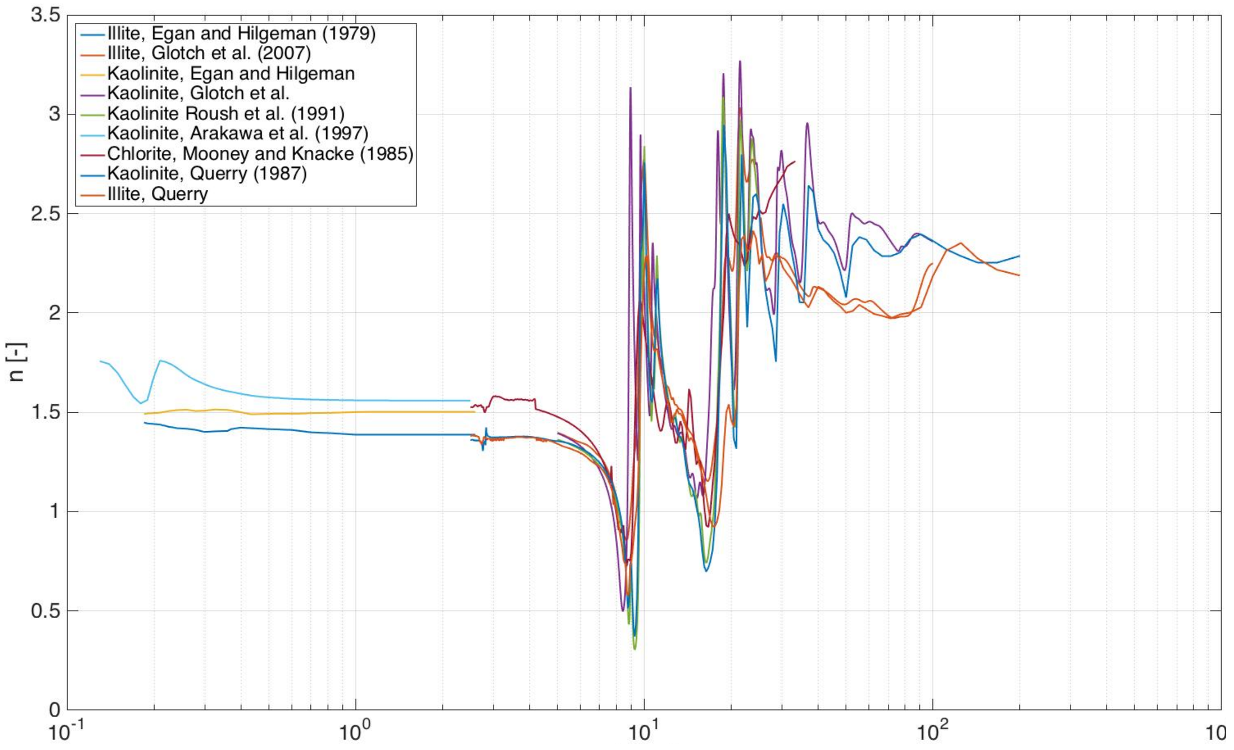
Effective Medium Refractive Index

- Common practice is to compute the refractive index of mineral dust via the **volume ratio** of its constituents.
- Here, the effective refractive index is calculated based on the method of Bruggeman (Ann. d. Phys. 1935):

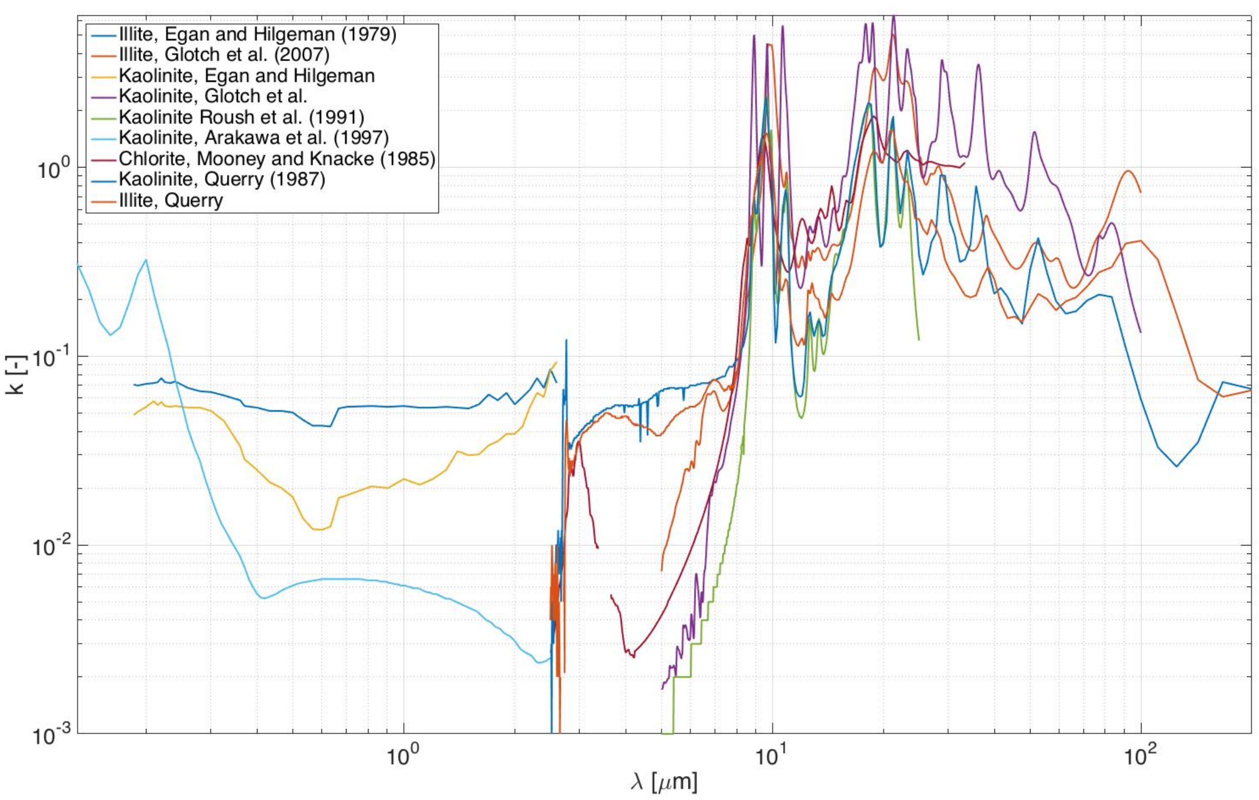
$$\sum_i f_i \frac{\varepsilon_i - \varepsilon_{eff}}{\varepsilon + 2\varepsilon_{eff}} = 0$$

Example: Silicates group

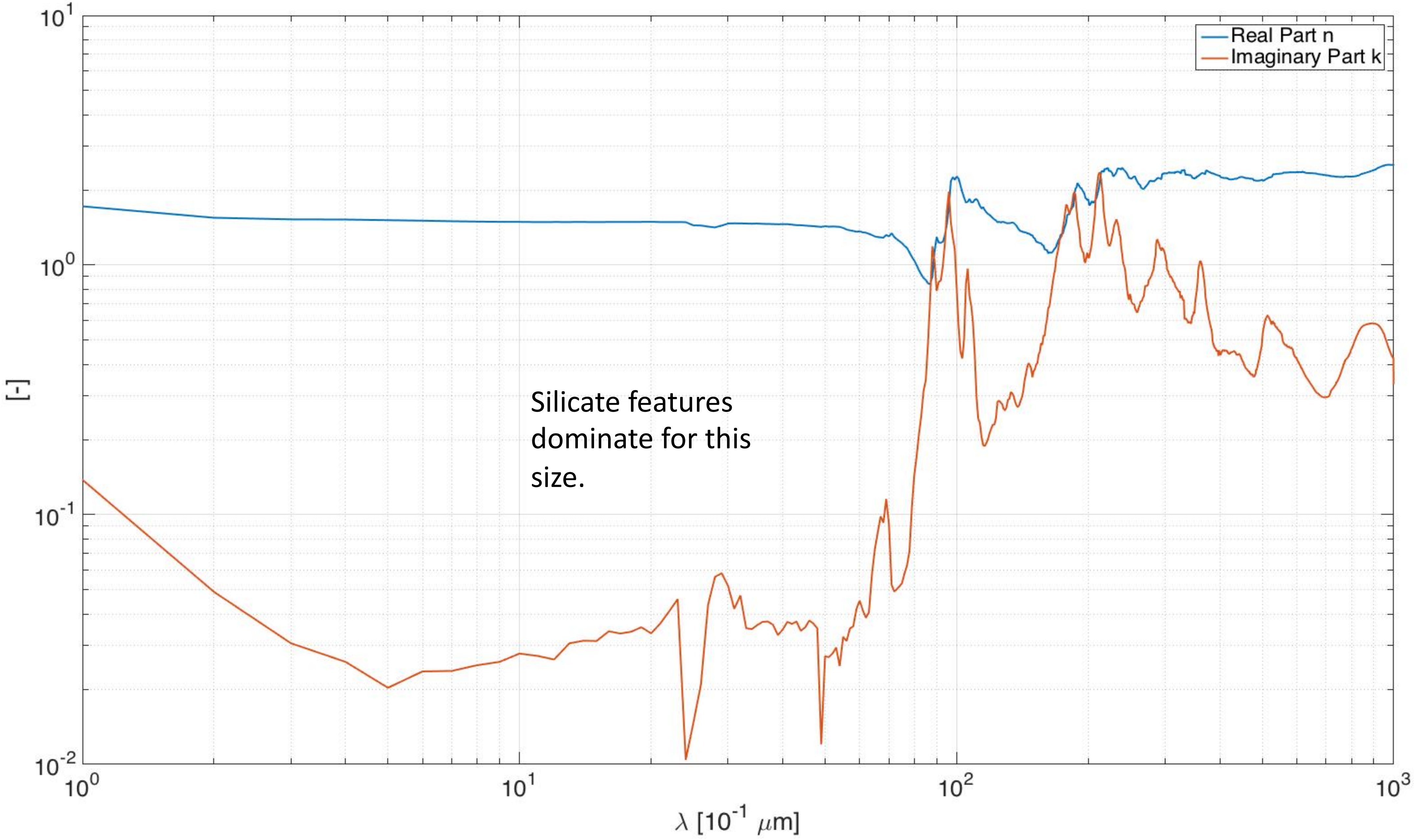
All databases for real part.



Imaginary part.



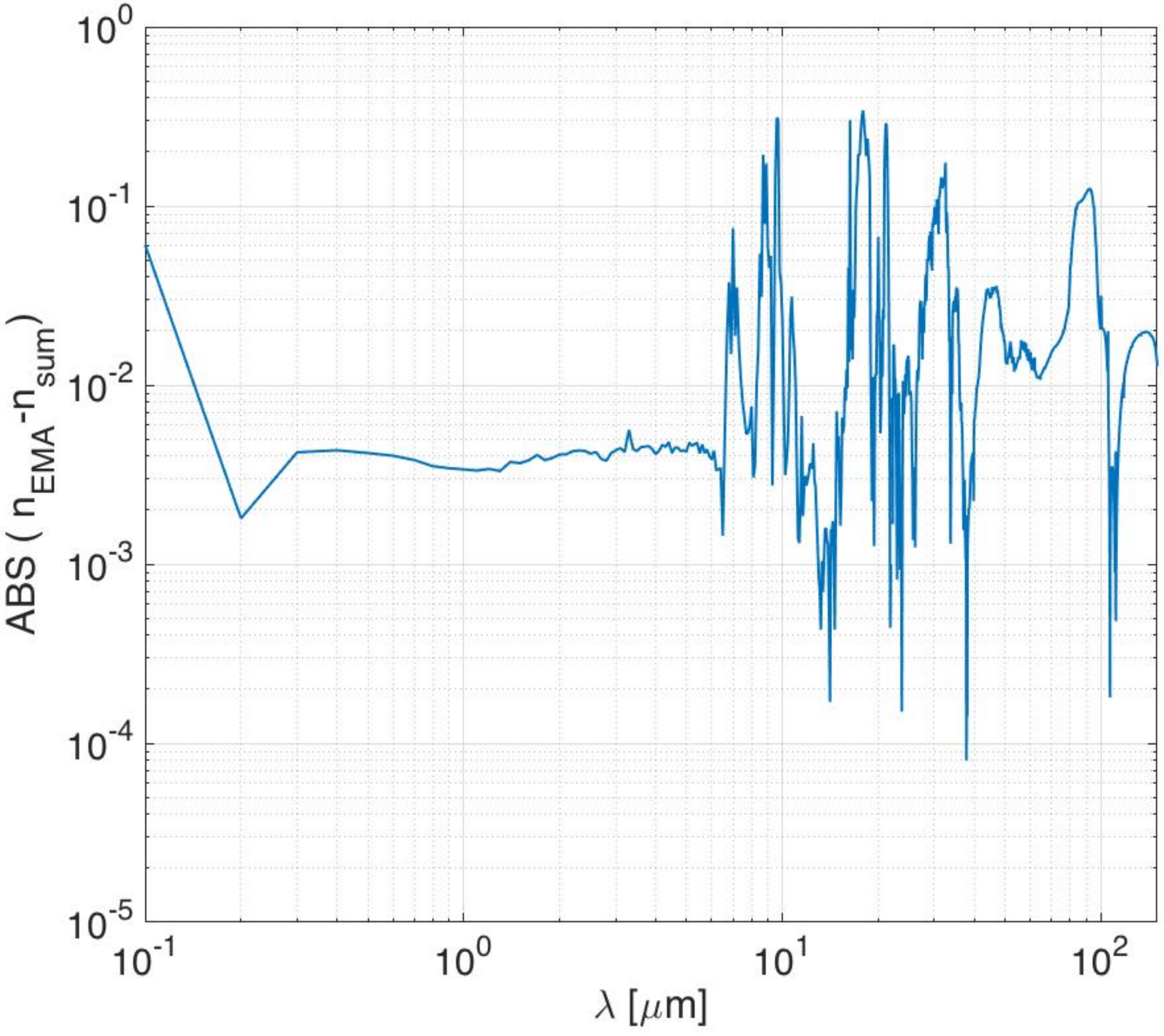
Effective Spectrum for size=0.1 μm



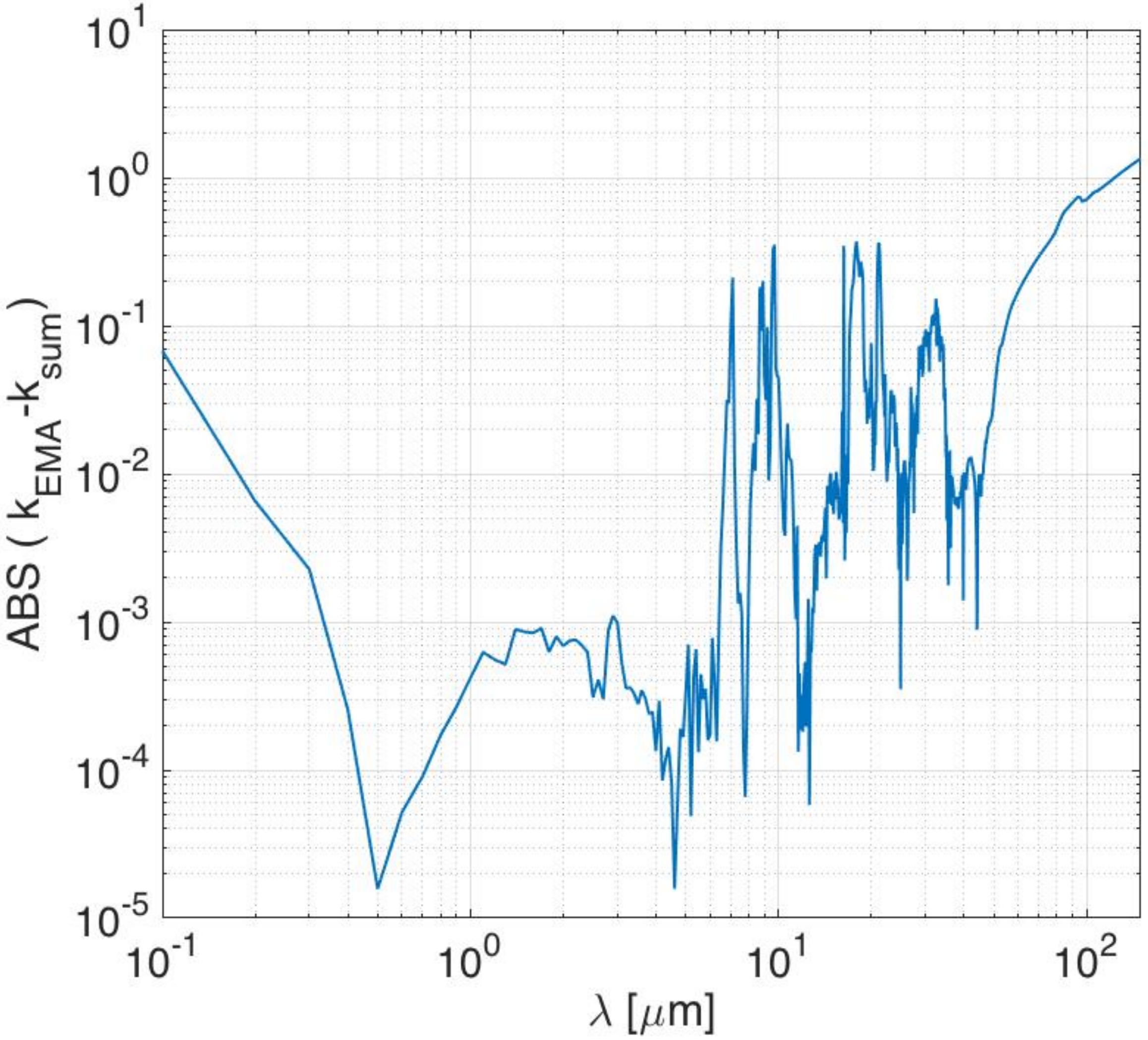
Silicate features dominate for this size.

Comparison to simple volumetric addition (size 0.1 µm)

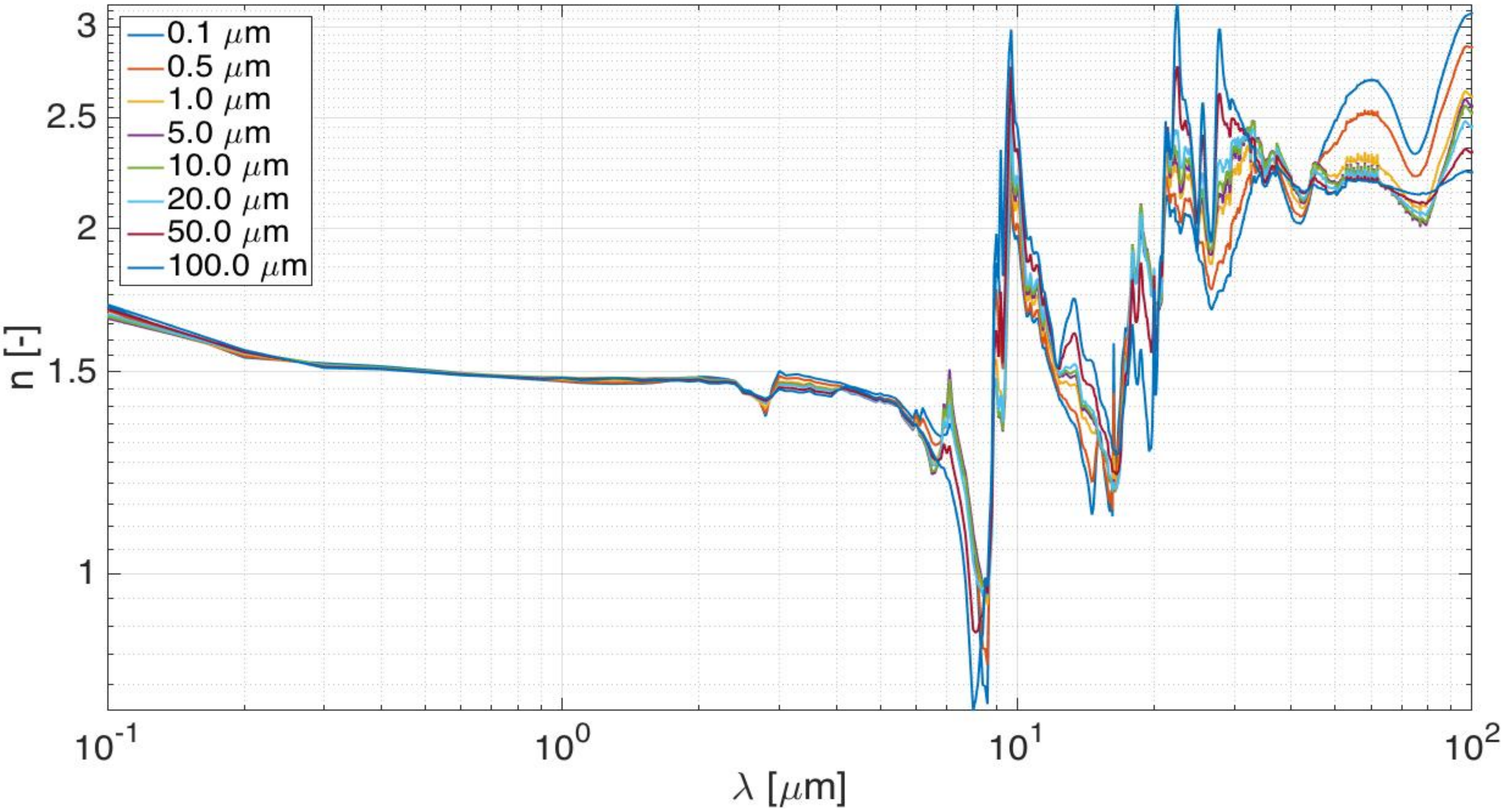
Real part.



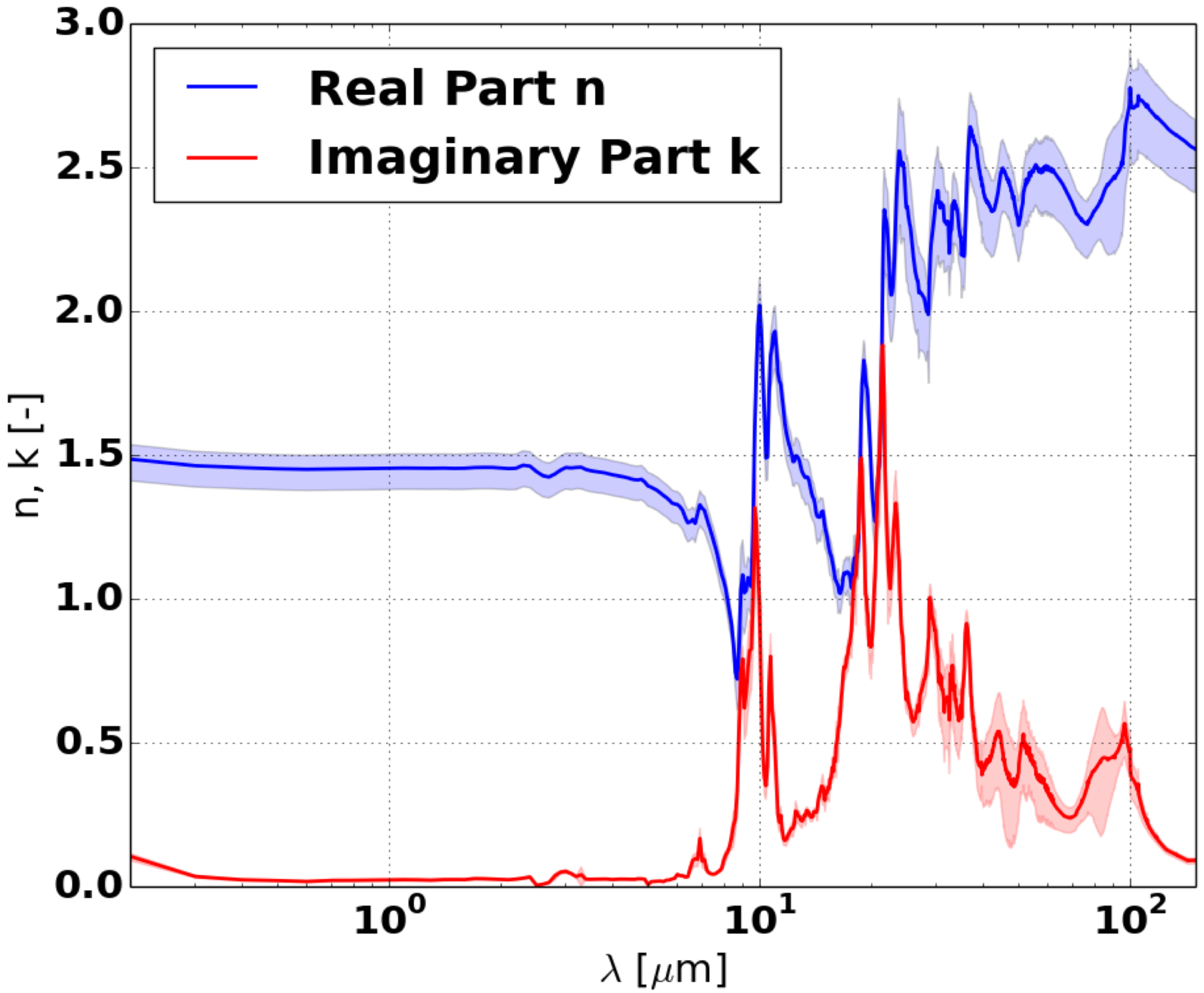
Imaginary part.



Effect of Dust Particle Size Variation



Size-Integrated Refractive Index



Bimodal particle number size distribution measured at Cap Verde used as weighting function.

Ensuring a Causal Spectrum

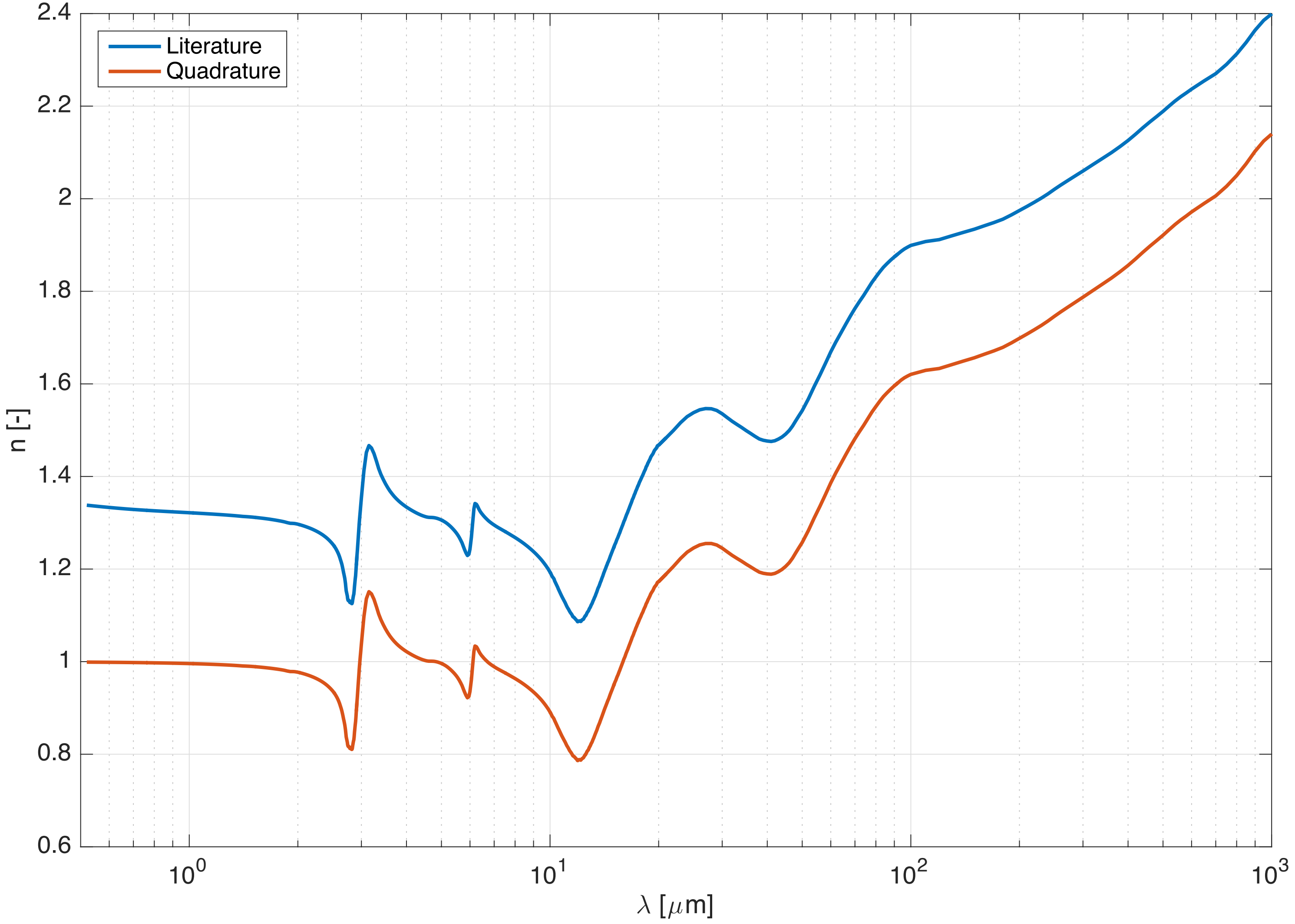
KRAMERS-KRONIG ANALYSIS

Kramers-Kronig Analysis of effective spectrum

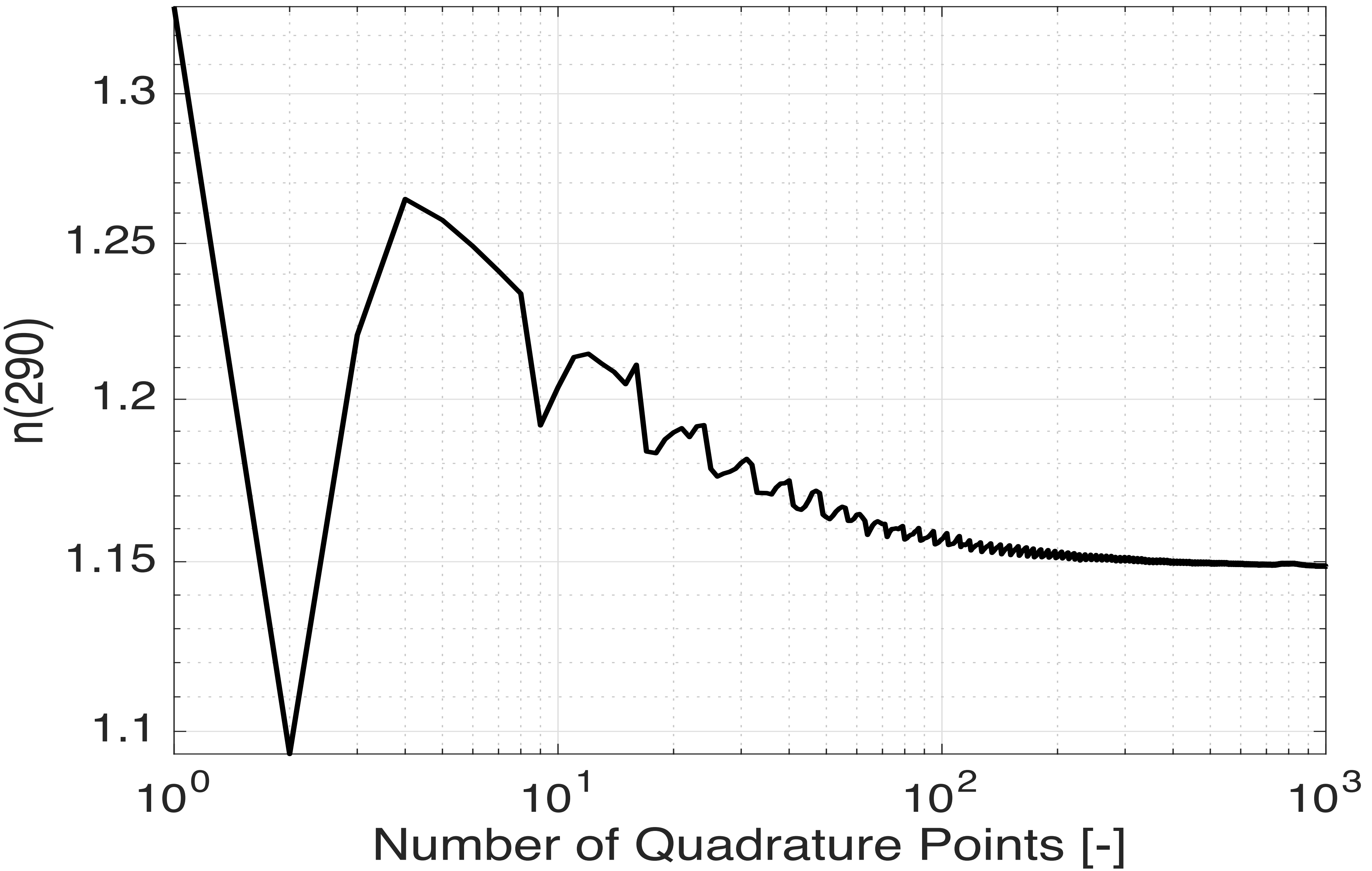
- Method based on Iwabuchi and Yang (2011), which is in turn based on S. G. Warren (1984).
- Enforce Cauchy's residue theorem to compute the real part of the refractive index using the trapezoidal rule and skip the singularity at ν.

$$n(\nu) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\mu^2 \cdot \kappa(\mu) - \nu \cdot \mu \cdot \kappa(\nu)}{\mu^2 - \nu^2} \, d\ln\mu$$

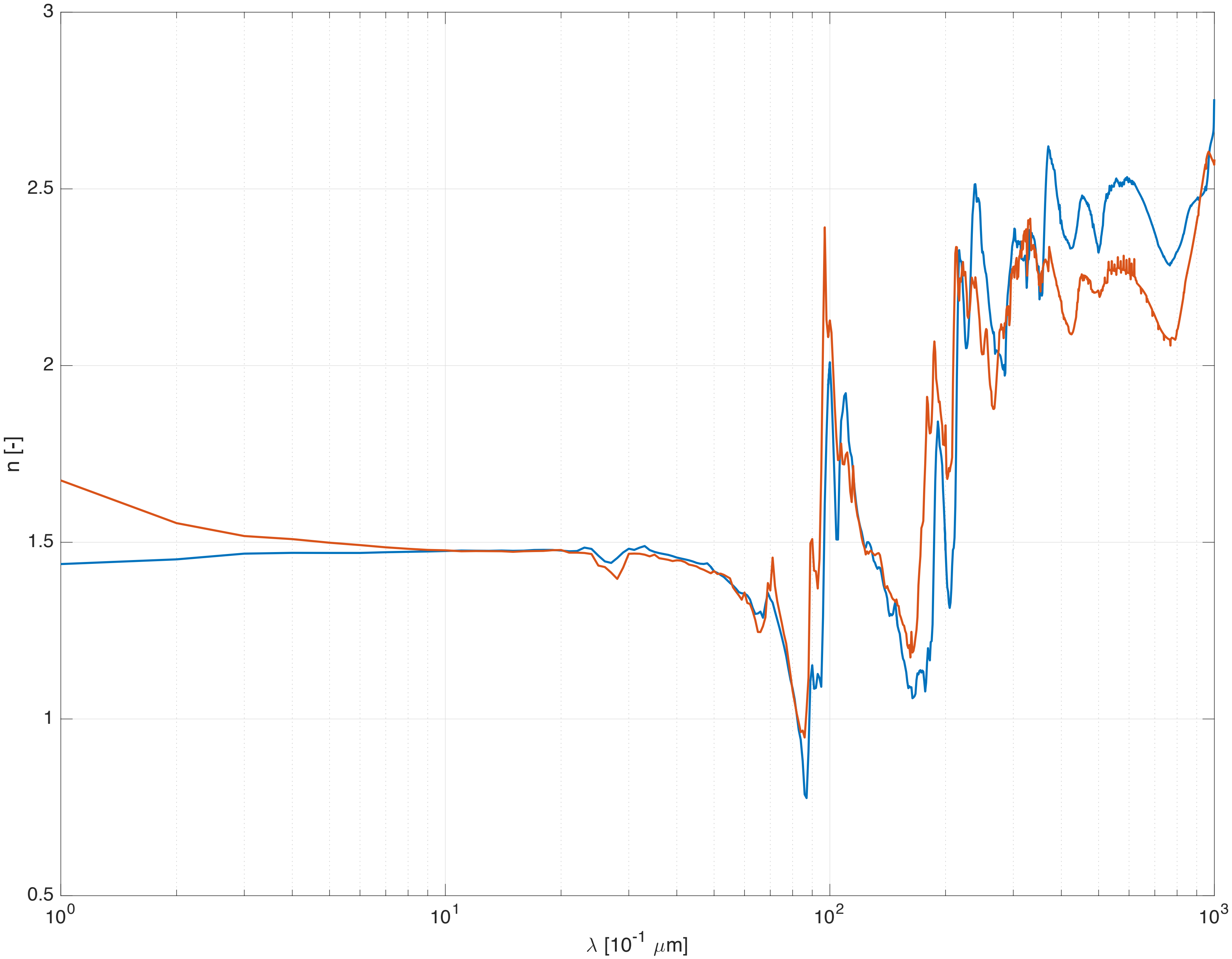
Hilbert transform validation for H_2O refractive index spectrum



Quadrature Convergence



Kramers-Kronig Analysis of effective spectrum



Local and Monte Carlo Sensitivity

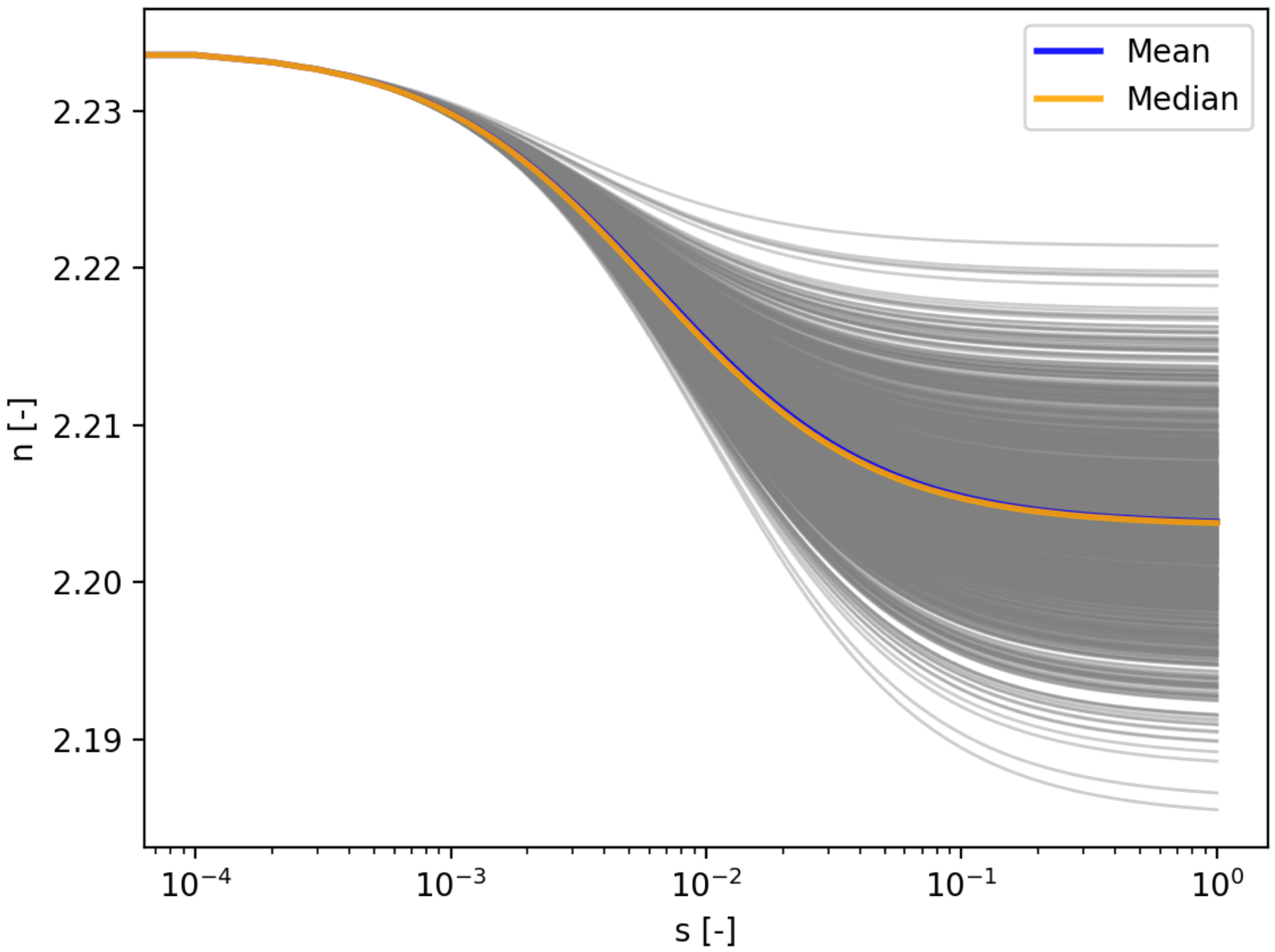
SENSITIVITY ANALYSIS

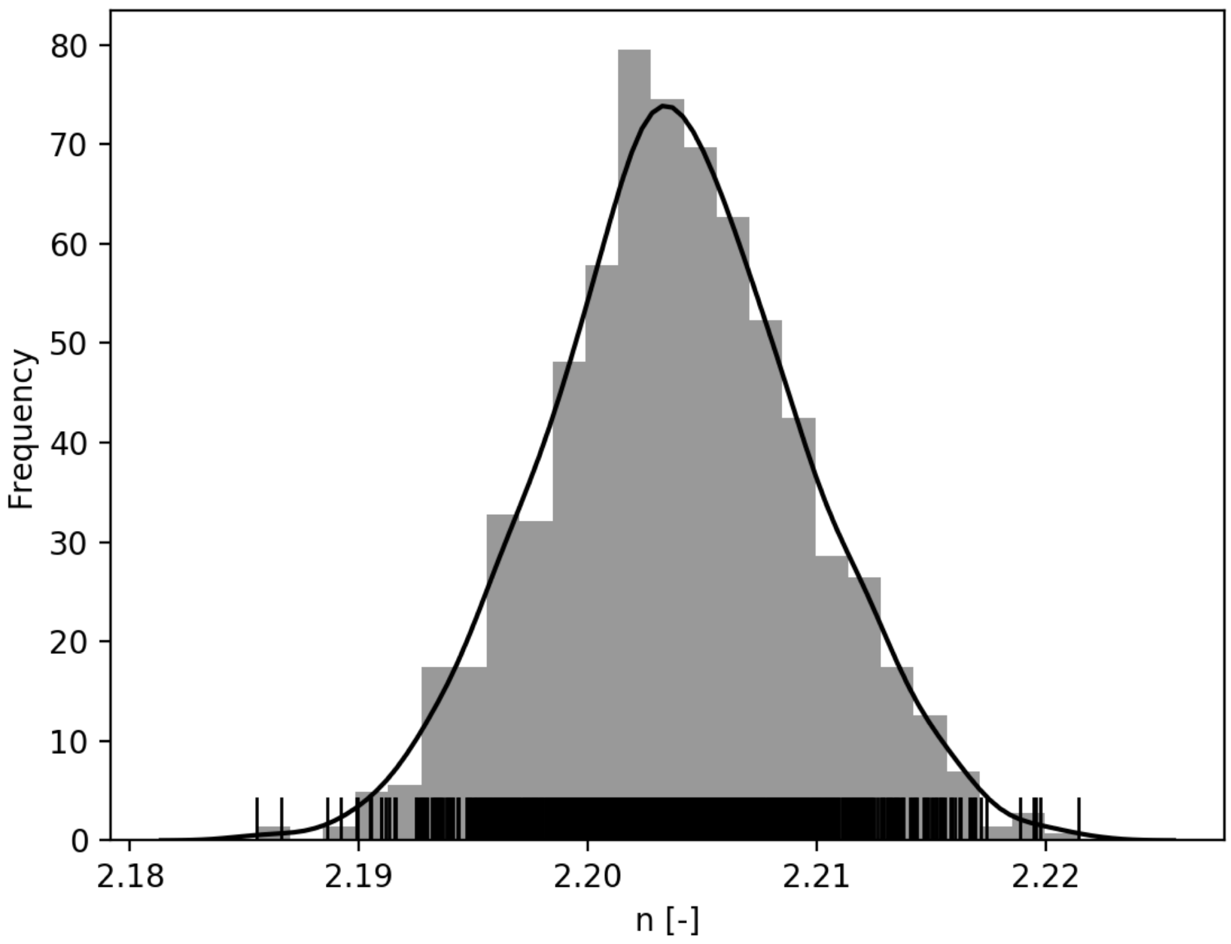
Bruggeman ODE

- A unique physical solution for a Bruggeman effective medium with an arbitrary number of components can be found via an ODE approach.
- This also provides an elegant framework for sensitivity analysis with respect to the ODE parameters (i.e. particle composition and components).

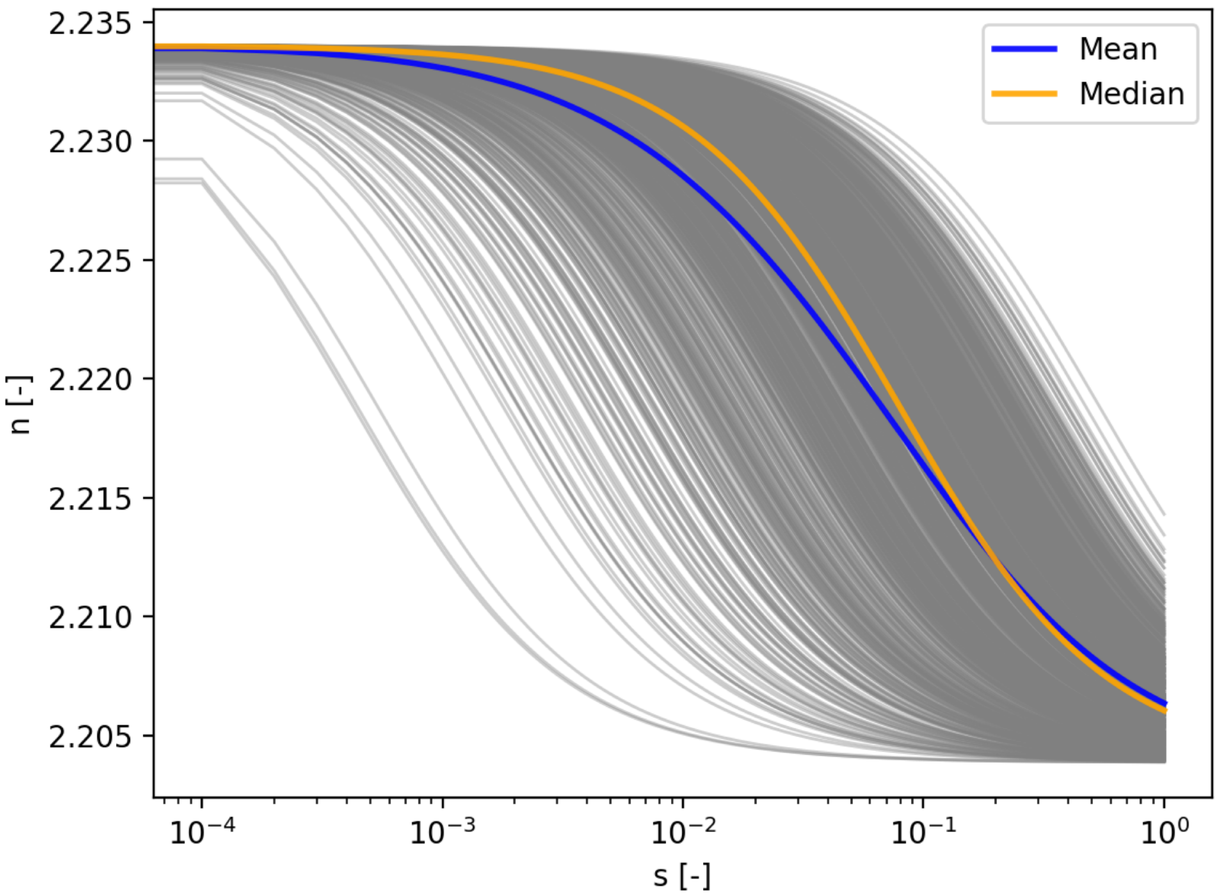
$$\frac{d\varepsilon_{eff}(s)}{ds} = \frac{1}{3} \cdot \frac{\sum_{j=2}^{N} f_j \frac{\varepsilon_j - \varepsilon_{eff}(s)}{\varepsilon_j + 2\varepsilon_{eff}(s)}}{\sum_{j=1}^{N} f_j(s) \frac{\varepsilon_j}{\left[\varepsilon_j + 2\varepsilon_{eff}(s)\right]^2}}$$

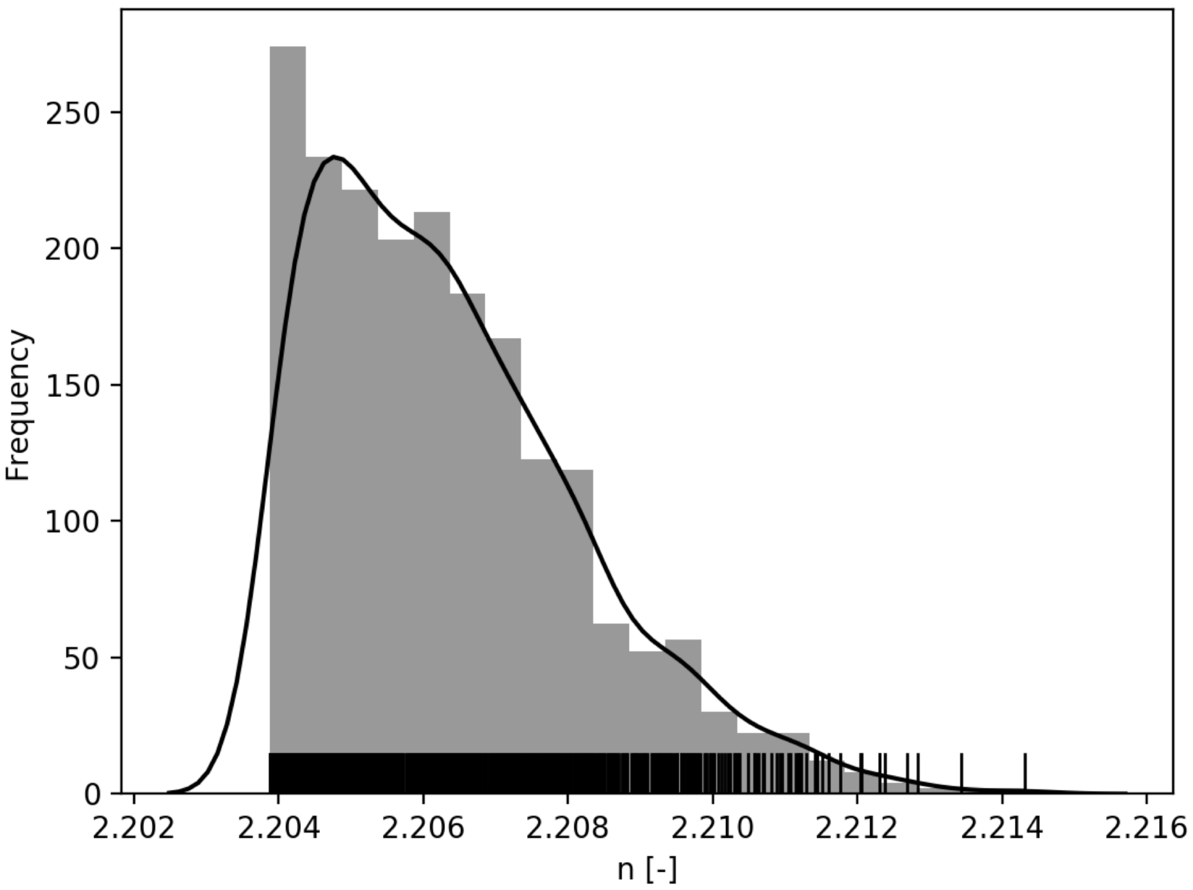
Monte Carlo Results: Composition



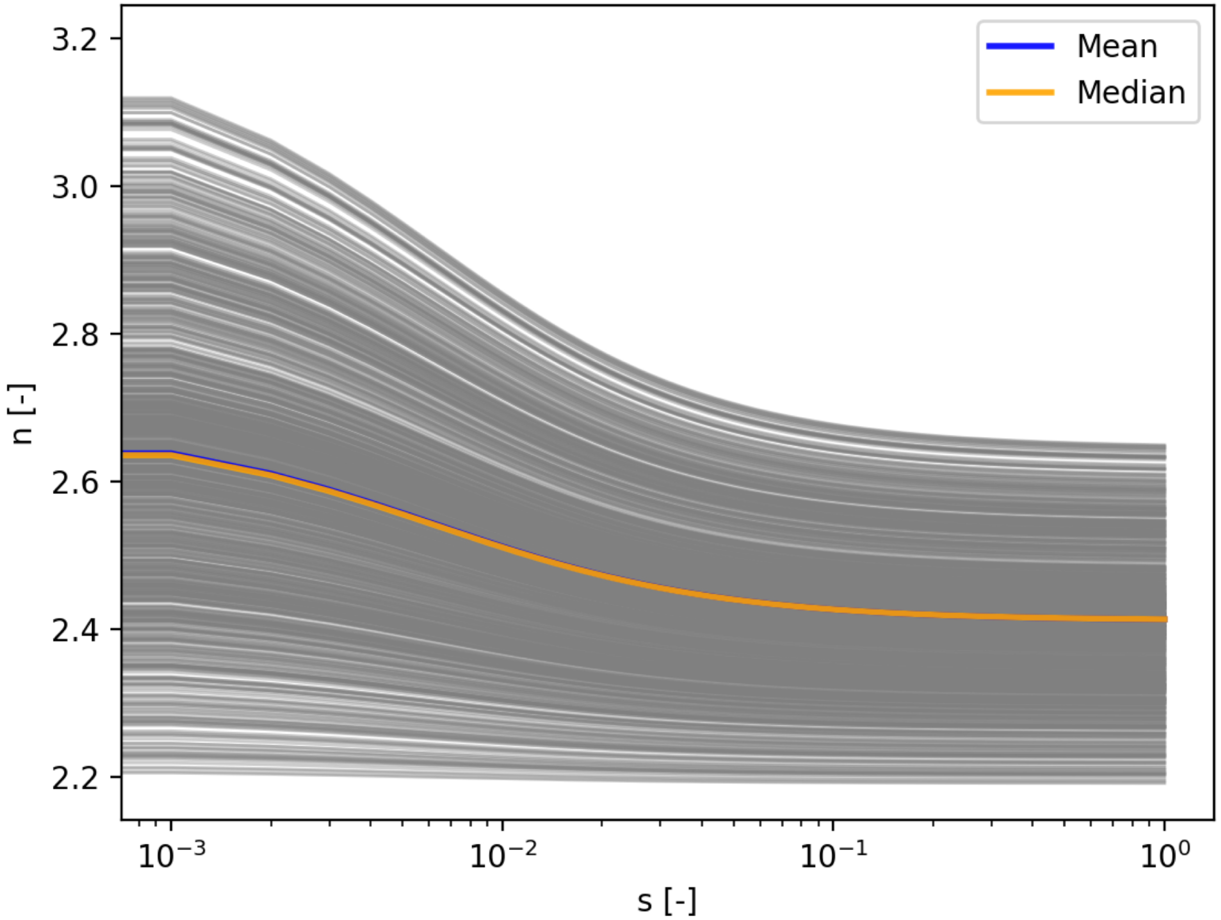


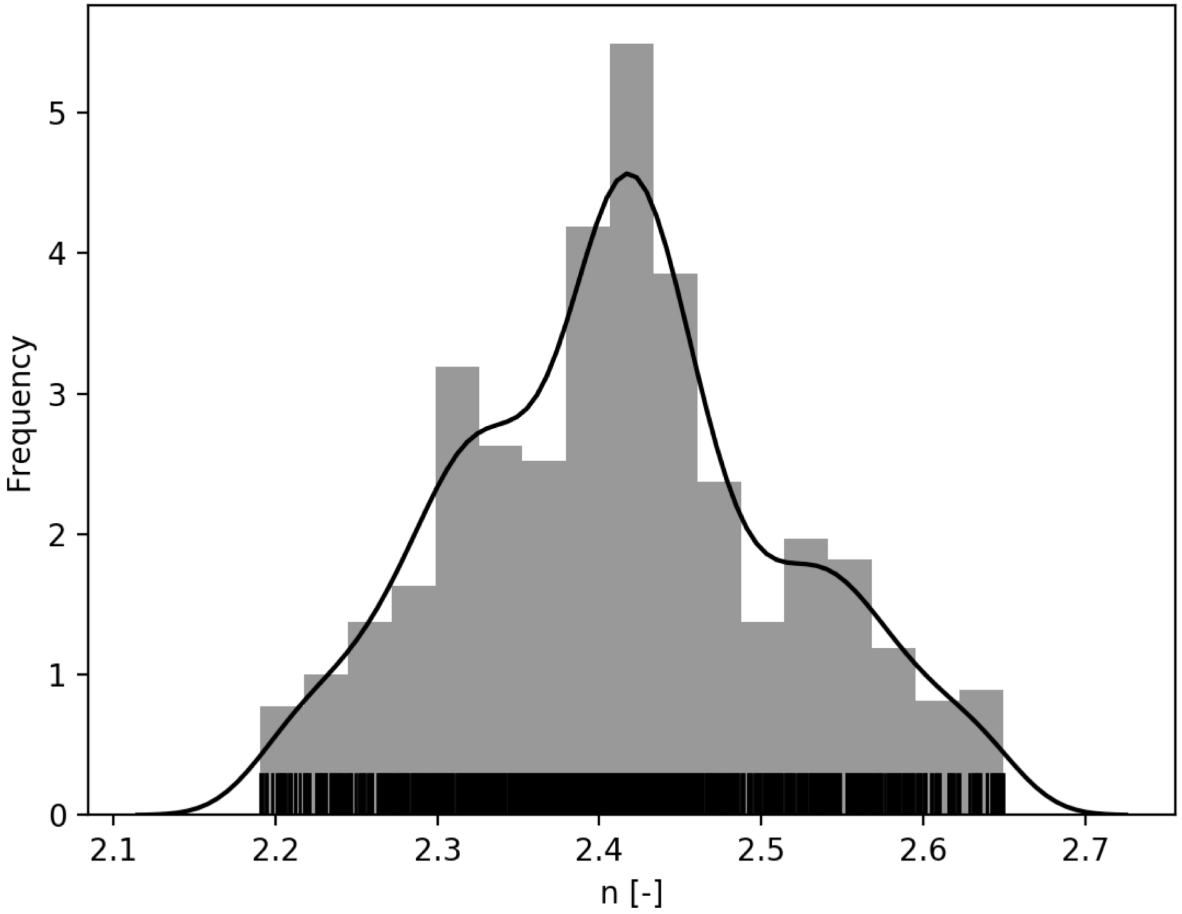
Monte Carlo Results: Composition





Monte Carlo Results: Component Index





Local Sensitivity

- Sensitivity ODE:

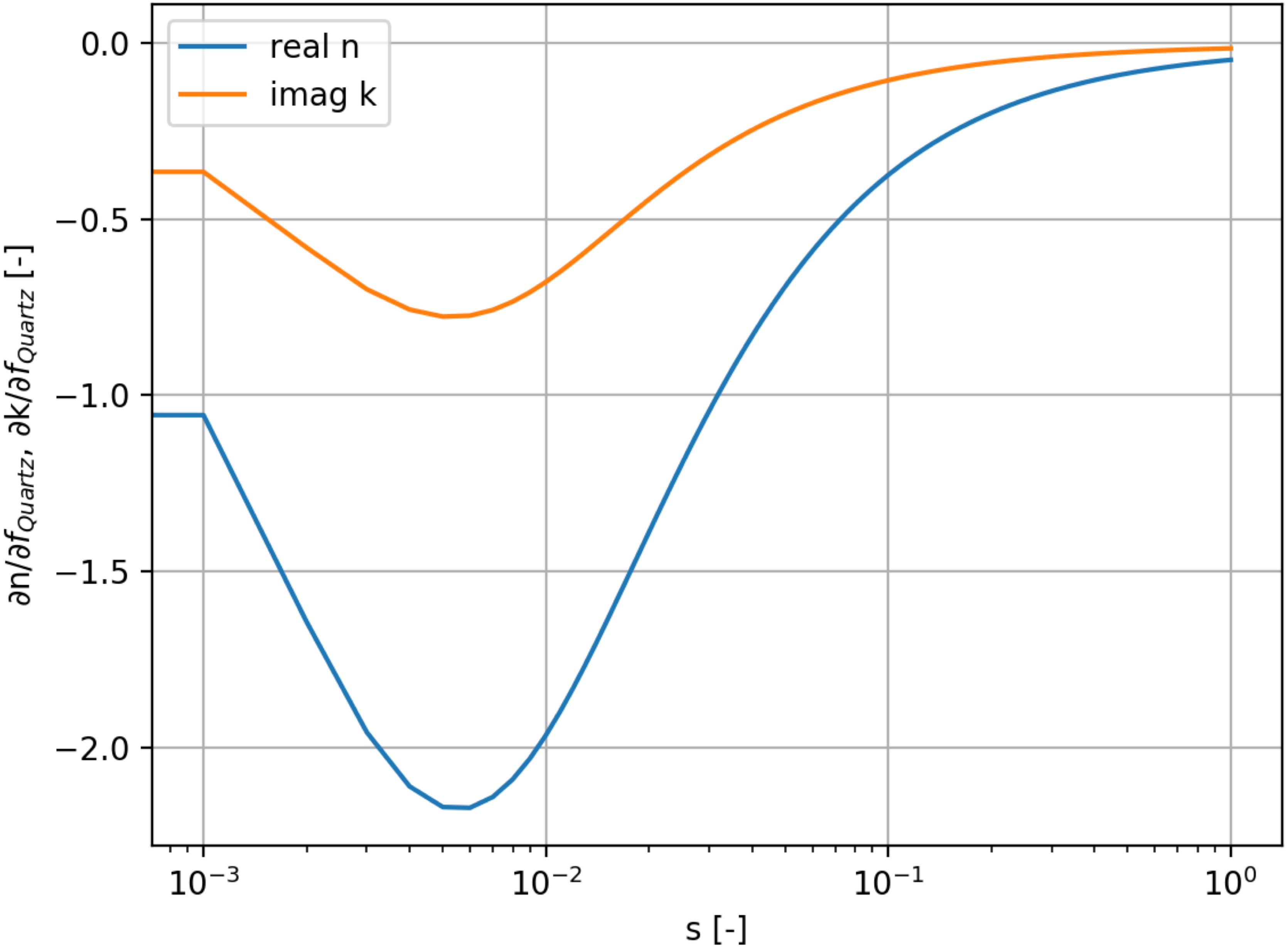
Composition:

$$\frac{d}{ds}\left(\frac{\partial \varepsilon_{eff}}{\partial f_j}\right) = \frac{\partial RHS}{\partial \varepsilon_{eff}} \cdot \frac{\partial \varepsilon_{eff}}{\partial f_j} + \frac{\partial RHS}{\partial f_j}$$

Component Index:

$$\frac{d}{ds}\left(\frac{\partial \varepsilon_{eff}}{\partial \varepsilon_j}\right) = \frac{\partial RHS}{\partial \varepsilon_{eff}} \cdot \frac{\partial \varepsilon_{eff}}{\partial \varepsilon_j} + \frac{\partial RHS}{\partial \varepsilon_j}$$

Local Sensitivity: Example



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Patrick G. Stegmann, Ping Yang

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