## 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

	WN	WL	N	к	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		D-11-+
	2100.00	4.7619	1.397	0.031	0.010	0.011	0.02810		Pellet.
	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		к
	2140.00	4.6729	1.400	0.033	0.010	0.011	0.02840		
	2150.00	4.6512	1.402	0.032	0.010	0.011	0.02875		0.100 0
	2160.00	4.6296	1.404	0.033	0.010	0.011	0.02895		0.114 0
	2180.00	4.5872	1.402	0.036	0.010	0.011	0.02890		0.087 0
	2190.00	4.5662	1.404	0.033	0.010	0.011	0.02900		0.092 0
	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		
	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		Table 8
	2250.00	4.4444	1.408	0.035	0.010	0.012	0.02945		
	2270.00	4.4053	1.409	0.031	0.009	0.012	0.02920		
	2280.00	4.3860	1.410	0.033	0.009	0.012	0.02965		WN
	2290.00	4.3668	1.409	0.033	0.009	0.012	0.02955		550 00
	2300.00	4.3478	1.409	0.031	0.009	0.012	0.02950		560.00
	2320.00	4.3103	1.411	0.031	0.009	0.012	0.02975		570.00
	2330.00	4.2918	1.413	0.030	0.009	0.012	0.03000		580.00
	2340.00	4.2735	1.415	0.031	0.009	0.012	0.03025		590.00
	2360.00	4.2373	1.414	0.033	0.009	0.012	0.03030		600.00
	2370.00	4.2194	1.416	0.032	0.009	0.012	0.03040		610.00
	2380.00	4.2017	1.415	0.033	0.009	0.012	0.03030		620.00
	2390.00	4.1841	1.416	0.033	0.009	0.012	0.03040		630.00
	2410.00	4.1494	1.417	0.028	0.009	0.012	0.03040		650.00
	2420.00	4.1322	1.421	0.031	0.009	0.012	0.03095		660.00
	2430.00	4.1152	1.419	0.034	0.009	0.012	0.03070		670.00
	2450.00	4.0816	1.421	0.031	0.009	0.012	0.03090		680.00
	2460.00	4.0650	1.422	0.033	0.009	0.012	0.03110		690.00
	2470.00	4.0486	1.420	0.034	0.009	0.012	0.03085		700.00
	2480.00	4.0323	1.421	0.033	0.009	0.012	0.03095		710.00
	2500.00	4.0000	1.422	0.033	0.009	0.012	0.03105		720.00
	2510.00	3.9841	1.421	0.033	0.009	0.012	0.03100		740.00
	2520.00	3.9683	1.422	0.034	0.009	0.012	0.03115		750.00
	2540.00	3.9370	1.422	0.032	0.009	0.012	0.03095		760.00
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		5			490.	00 2	88		860.00
		3			500.	00 2	80		870.00
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		ŝ			520.	00 1	22		890.00
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Table 8. Montmorillonite Péllet.

	3													
		Table 8.	Montmori	llonite	Pellet.		F	AGE	3					
	ž.	WN	WL	N	ĸ	DN	DK	F	ર					
DN		1050 00	0 5239	1 829	1 802	0 077	0.019	0.95	7090					
0.022		1060.00	9 4340	1 331	1.032	0.077	0.018	0.3		-				
0 012	25	1070.00	9.3458	0.89										
0 011		1080.00	9.2593	0.70										
0 011		1090.00	9.1743	0.71										
0.011		1100.00	9.0909	0.79										
	1. A A A A A A A A A A A A A A A A A A A	1110.00	9.0090	0.88			Table	8.	Montmori	llonite	Pellet.		P	AGE 4
	<b>X</b>	1120.00	8.9286	0.89										
	8	1130.00	8.8496	0.79										
8. Mo	n	1140.00	8.7719	0.71			WN		WL	N	ĸ	DN	DK	R
		1150.00	8.6957	0.67						••				
		1160.00	8.6207	0.67			1550 0	0	6 4516	1 304	0.051	0 011	0 009	0 01820
	WIE	1170.00	8.5470	0.70			1560.0	õ	6 4103	1 307	0.051	0 011	0.010	0 01860
	8	1180.00	8.4746	0.72			1570.0	ŏ	6 3694	1 212	0.048	0 011	0.010	0 01010
0 18.	1 1	1190.00	8.4034	0.77			1590.0	õ	6 3291	1 319	0.050	0 011	0.010	0 01970
0 17.	8 💱	1200.00	8.3333	0.83			1500.0	č	6 2903	1 321	0.050	0.011	0.010	0.01970
0 17.	5 🙀	1210.00	8.2645	0.88			1590.0	č	6.2693	1 325	0.050	0.011	0.010	0.02000
0 17.	2	1220.00	8.1967	0.92			1600.0	2	6.2500	1.325	0.051	0.011	0.010	0.02040
0 16.	9.23	1230.00	8.1301	0.90			1610.0	~	0.2112	1.329	0.050	0.011	0.010	0.02085
0 16.	6	1250.00	8.0045	1.03			1620.0	0	6.1728	1.331	0.054	0.011	0.010	0.02105
0 16.	3:	1260.00	7.9365	1.05			1630.0	0	6.1350	1.330	0.051	0.011	0.010	0.02095
0 16.	1.	1270.00	7.8740	1.08			1640.0	0	6.0976	1.335	0.050	0.011	0.010	0.02140
0 15.	8	1280.00	7.8125	1.10			1650.0	0	6.0606	1.337	0.049	0.011	0.010	0.02165
0 15.	6.0	1290.00	7.7519	1.11			1660.0	0	6.0241	1.341	0.048	0.011	0.010	0.02210
0 15.	3.00	1300.00	7.6923	1.12!			1670.0	0	5.9880	1.346	0.048	0.011	0.010	0.02265
0 15.	1.0	1310.00	7.6336	1.13			1680.0	0	5.9524	1.353	0.053	0.011	0.011	0.02350
0 14.	9 8	1320.00	7.5758	1.15			1690.0	0	5.9172	1.352	0.063	0.011	0.011	0.02360
14.	7	1330.00	7.5188	1.175			1700.0	0	5.8824	1.344	0.064	0.011	0.011	0.02270
14.	4	1340.00	7.4627	1.18			1710.0	0	5.8480	1.343	0.061	0.011	0.011	0.02250
14.	2 3	1350.00	7.4074	1.19			1720.0	0	5.8140	1.340	0.059	0.011	0.010	0.02215
14.		1360.00	7.3529	1.21			1730.0	0	5.7803	1.338	0.053	0.011	0.010	0.02185
13.		1370.00	7.2993	1.22			1740.0	0	5.7471	1.341	0.048	0.011	0.010	0.02205
0 13.	6 0	1380.00	7.2464	1.22			1750.0	0	5.7143	1.345	0.046	0.010	0.010	0.02240
0 13	3 4	1390.00	7.1942	1.23			1760.0	0	5.6818	1.347	0.043	0.010	0.010	0.02260
0 13	1 1	1410.00	7.0022	1.24			1770.0	0	5.6497	1.352	0.041	0.010	0.010	0.02315
0 12.	9.0	1420.00	7.0423	1.24			1780.0	0	5.6180	1.355	0.042	0.010	0.010	0.02345
0 12.	8 8	1430.00	6.9930	1.25			1790.0	0	5.5866	1.358	0.041	0.010	0.010	0.02375
0 12.	6 8	1440.00	6.9444	1.26			1800.0	ō	5.5556	1.359	0.043	0.010	0.010	0.02395
0 12.	5 2	1450.00	6.8966	1.26			1810.0	0	5.5249	1.361	0.041	0.010	0.010	0.02410
0 12.	31	1460.00	6.8493	1.26			1820 0	0	5.4945	1.362	0.042	0.010	0.011	0.02430
0 12.	1	1470.00	6.8027	1.26 {			1830 0	ň	5 4645	1 363	0.040	0 010	0 011	0 02430
0 12.	0.00	1480.00	6.7568	1.27			1840.0	ŏ	5 4348	1 367	0.040	0 010	0.011	0.02480
0 11.	9 8	1490.00	6.7114	1.28			1950.0		5 4054	1 369	0.042	0.010	0.011	0.02400
0 11.	7 0	1500.00	6.6667	1.28			1850.0		5.3763	1.300	0.041	0.010	0.011	0.02490
0 11.	6	1510.00	6.6225	1.28			1070 0	6	5.3/03	1 270	0.041	0.010	0.011	0.02403
0 11.	4	1520.00	6.5789	1.29			1870.0		5.3476	1.370	0.041	0.010	0.011	0.02510
0 11.	3 8	1530.00	6.5359	1.29			1880.0	0	5.3191	1.370	0.040	0.010	0.011	0.02515
0 11.	2	1540.00	6.4935	1.29			1890.0	0	5.2910	1.372	0.040	0.010	0.011	0.02530
0 11.	1 8			R			1900.0	0	5.2632	1.372	0.039	0.010	0.011	0.02530
0 10.	9			8			1910.0	0	5.2356	1.374	0.038	0.010	0.011	0.02555
0 10.	8			1			1920.0	0	5.2083	1.375	0.038	0.010	0.011	0.02570
10.				l l			1930.0	0	5.1813	1.376	0.038	0.010	0.011	0.02575
10.				0000000			1940.0	0	5.1546	1.378	0.037	0.010	0.011	0.02595
10.							1950.0	0	5,1282	1.379	0.038	0.010	0.011	0.02615
10.	4167 2.009 0.1		0.034	0 1221			1960.0	0	5.1020	1.379	0.037	0.010	0.011	0.02610

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#### **Optical Character Recognition for Automatic Database Acquisition**

- Rarely refractive index values are available as ٠ **Dispersion Relations.**
- Vast data tables are preferred by authors. ٠
- 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 ٠ Recognition (OCR) code has been developed in Python
- OCR code fails if text misalignment is too large, ٠ e.g. for books, but provides a huge speed-up and considerable increase in reliability in many other cases, e.g. for PDFs.



TABLE 1 (Continued) Calcium Carbonate (Calcius)								
1-1	μm	no	k k					
71.6	0.1690			n <sub>e</sub>				
78.0	0.1698	2.34	0.0025 [4]					
79.5	0.1710		0.035 [1]	1.69				
1.5	0.1722	2.26	0.0066 [4]		0.0			
13.5	0.1730		0.018 [1]	1.68	0.0			
4.9	0.1746	2.20	0.0041 [4]		0.0			
12.9	0.1750		0.006 [1]	1.67				
97.2	0.1770		0.0029 [4]		0.0			
8.4	0.1771	2.14	0.0027	and the second se	0.0			
5.9	0.1790		0.0022	1.66				
1.8	0.1797	2.09	0.0033		0.0			
18.6	0.1810		0.0027	1.64				
5.3	0.1823	2.05	0.0057	1.63	0.0			
4.8	0.1830		0.0039	1.0.3	0.0			
54.1	0.1850		0.0041		0.0			
8.7	0.1851	2.02	0.0011	1.62	0.0			
5.9	0.1870		0.0036	1.02	0.0			
0.1	0.1890		0.0027		0.0			
6.0	0.1910		0.0016		0.0			
3.8	0.19899			1.57796 [6]				
7.5	0.20009	1.90284 [6]		1.57649				
6.9	0.20447	1.88242		1.57081				
7.0	0.20821	1.86733		1.56640				
6.3	0.20988	1.8608110[7]						
5.9	0.21108	1.85692 [6]		1.56327				
0.9	0.21445	1.84558		1.55976				
		1.8458240[7]		1.5599225 [7]				
0.5	0.21944	1.8307980		1.5551219				
6.4	0.21946	1.83075 [6]		1.55105				
2.9	0.22400	1.81890		1 5491444 171				
7.6	0.22651	1.8130351 [7]		1.5455001				
2.2	0.23110	1.8023942		1.54541 [6]				
5.8	0.23129	1.80233 [6]		1.53782				
4.5	0.24281	1.78111		1.5373101 [7]				
5.4	0.24459	1.7796645[7]		1.53358 [6]				
6.8	0.25033	1.76968 [0]		1.5301212[7]				
3.3	0.25731	1.7605000[7]		1.53005 [6]				
2.6	0.25732	1.76038 [0]		1.52736				
3.9	0.26320	1.75345		1.52547				
7.8	0.26761	1.74804		1.5226617				
	0.27487	1.7413041[1]		1.52261 [6]				
		1.74139 [0]		1.52018				
	0.28164	1 72774		1.51705				
		1 7195881 [7]		1.5136464 [7]				
	0.30342	1 71657 [6]		1.51140				
		1 71425		Latitu				

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2.78 2.74 ~ 2.61...

% (str(X.dtype), format)) TypeError: Mismatch between array dtype ('|S1') and format specifier ('st.18e') stegmann@atmolan36: esser\$ python Ea Tesseract Open Source OCR Engine v3.04.01 with Leptonica Warning in pixReadMemPng: work-around: writing to a temp file =====output======

pstegmann@atmolap36:~/workspace/Python\_dev/OCR\_with\_Python/pytesser\$ python Ea: Tesseract Open Source OCR Engine v3.04.01 with Leptonica Warning in pixReadMemPng: work-around: writing to a temp file Error in pixGenHalftoneMask: pix too small: w = 77, h = 1439 Detected 3 diacritics =====output======

pstegmann@atmolap36:~/workspace/Python\_dev/OCR\_with\_Python/pytesser\$ python Ea Tesseract Open Source OCR Engine v3.04.01 with Leptonica Warning in pixReadMemPng: work-around: writing to a temp file ====output======

pstegmann@atmolap36:~/workspace/Python\_dev/OCR\_with\_Python/pytesser\$ python Ea Tesseract Open Source OCR Engine v3.04.01 with Leptonica Warning in pixReadMemPng: work-around: writing to a temp file Error in pixGenHalftoneMask: pix too small: w = 88, h = 1462 ====output======

0.751 I



Dust composition is modeled based on a size-dependent composition

### S/A DUST GROUP MODEL



### **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.



Data base acquisition status

### REFRACTIVE INDEX SPECTRA OF INDIVIDUAL MINERALS

#### Quartz group



#### All databases for real part.

Imaginary part.

### Quartz group (moving average filter)



### Silicates group



#### All databases for real part.

### Carbonates group

#### All databases for real part. - Ivlev and Popova (1972) - Querry et al. (1978) - Long et al. (1993) - Tropf (1998) 10 Jarzembski et al. (2003) Jurewicz (2003) 10<sup>0</sup> 10-1 10-2 k [-] [-] u 10-3 10 10 - Ivlev and Popova (1972) - Querry et al. (1978) - Long et al. (1993) - Tropf (1998) - Jarzembski et al. (2003) - Jurewicz (2003) 10<sup>-1</sup> 10 10<sup>2</sup> 10 10<sup>0</sup> 10<sup>1</sup> $10^{3}$ 10<sup>4</sup> 10<sup>5</sup> 10-1 10<sup>0</sup> 10<sup>1</sup> 10<sup>2</sup> 10<sup>3</sup> 10<sup>4</sup> 10<sup>5</sup> $\lambda$ [ $\mu$ m] $\lambda \, [\mu m]$

#### **Imaginary part**

#### Sulphates group



Imaginary part.

### Iron oxides group

Imaginary part.

 $\lambda [\mu m]$ 



#### All databases for real 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



#### Comparison to simple volumetric addition (size 0.1 µm)



#### 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 v.

$$n(v) = 1 + \frac{2}{\pi} P \int_{0}^{\infty} \frac{\mu^2 \cdot \kappa(\mu) - v \cdot \mu \cdot \kappa(v)}{\mu^2 - v^2} d\ln \mu$$

# Hilbert transform validation for H<sub>2</sub>O 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).  $\sum_{n=1}^{N} \frac{\varepsilon_{n} \varepsilon_{n}(s)}{\varepsilon_{n} \varepsilon_{n}(s)}$

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

#### Monte Carlo Results: Composition



#### Monte Carlo Results: Composition



#### Monte Carlo Results: Component Index



#### Local Sensitivity

• Sensitivity ODE:

Composition:

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

Component Index:

#### Local Sensitivity: Example



### Online content



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### A regional, size-dependent, and causal effective medium model for Asian and Saharan mineral dust refractive index spectra

Patrick G. Stegmann  $\stackrel{\circ}{\sim} \boxtimes$ , Ping Yang

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https://doi.org/10.1016/j.jaerosci.2017.10.003

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