Modeling Optical Extinction Spectra of Polystyrene Beads in Water

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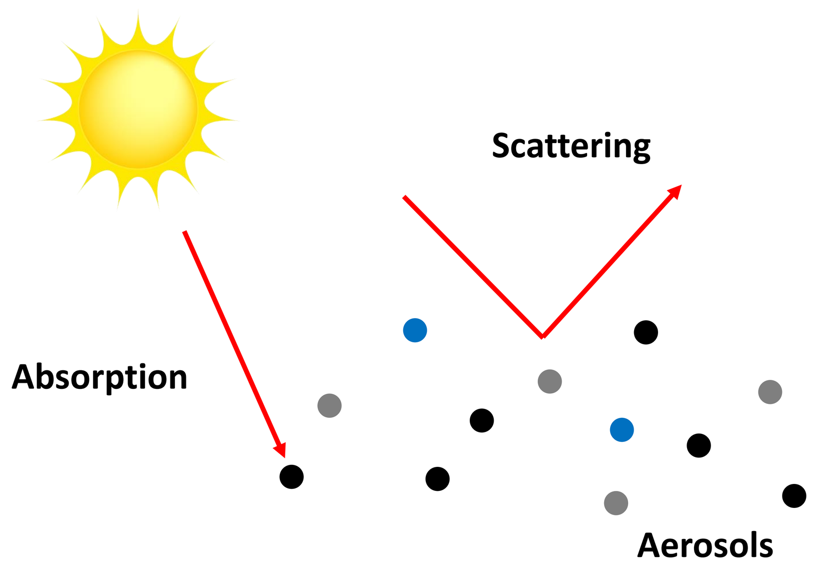
Introduction

To model the global climate, it is critical to understand how light interacts with particles in the atmosphere. Extinction spectra have been measured and simulated for a model system consisting of polystyrene beads in water. These beads have sizes comparable to atmospheric aerosols and can be dyed to mimic the properties of soot. Once the simulation is validated by comparing optimized simulation parameters to nominal particle properties, it can be used to study soot aerosols. We show that our simulation program can be fit to measured data to return reasonable values for the size and optical properties of this model system.



Polystyrene beads are commonly used as a model aerosol. To use them to model scattering and absorption from real aerosols, we need to know the refractive index of the beads. However:

- Many literature sources report slightly different results for the refractive index
- The refractive index is difficult to measure for wavelengths below 265 nm due to absorption
- The absorption introduces a change to the refractive index known as *anomalous dispersion*
- This anomalous dispersion is complicated and hard to model
- Scattering theory offers us the means to measure the refractive in these regions

Simulation Program

Mie scattering theory dictates that the amount of light scattered by a particle depends on the radius of the particle and the refractive index relative to the medium. A simulation program was created in MATLAB to calculate the amount of light lost to scattering using Mie scattering calculations. These theoretical spectra could then be fit to measured extinction spectra in order to determine best fit values for particle parameters such as the refractive index. Since scattering is very sensitive to changes in refractive index, this method allows us to probe the complicated behavior of the refractive index of Polystyrene below 265 nm.

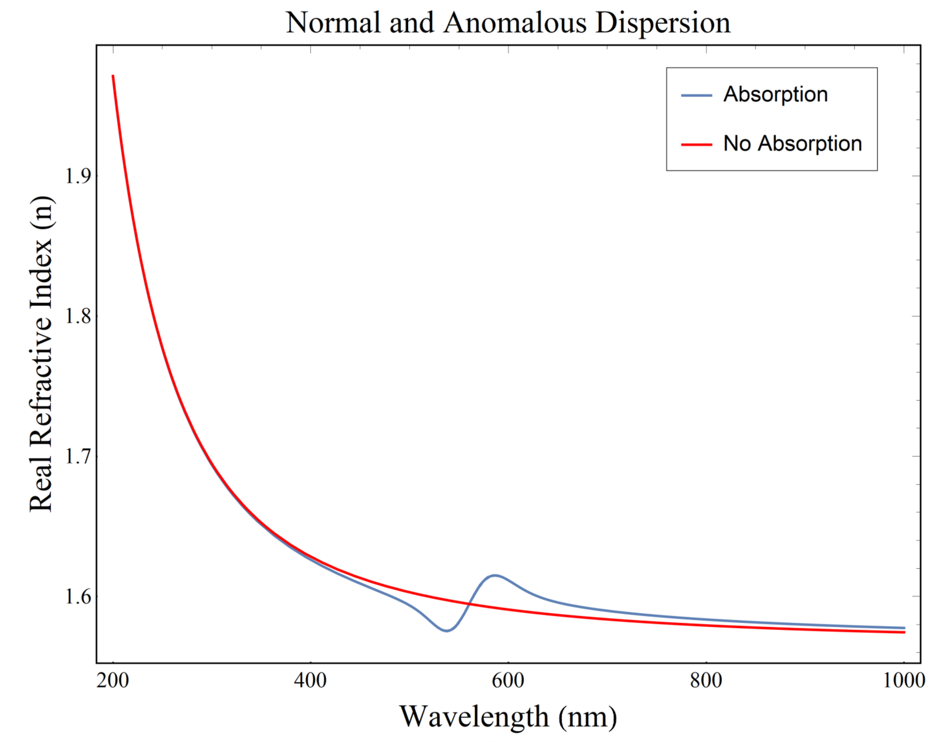
Scattering and Refractive Index

The refractive index as a function of the incident wavelength for materials such as polystyrene takes the form of (1), where κ represents the amount of absorption and Δn the resulting anomalous dispersion. If we can determine some empirical function α that fits the absorption we see in the scattering data, these terms can be determined using (2) and (3).

$$\tilde{n} = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} + \Delta n + i\kappa \quad (1)$$

$$\kappa = \alpha \frac{c}{2\omega} \quad (2)$$

$$\Delta n = \int_0^\infty \frac{\alpha(\omega')}{(\omega - \omega')^2} d\omega' \quad (3)$$

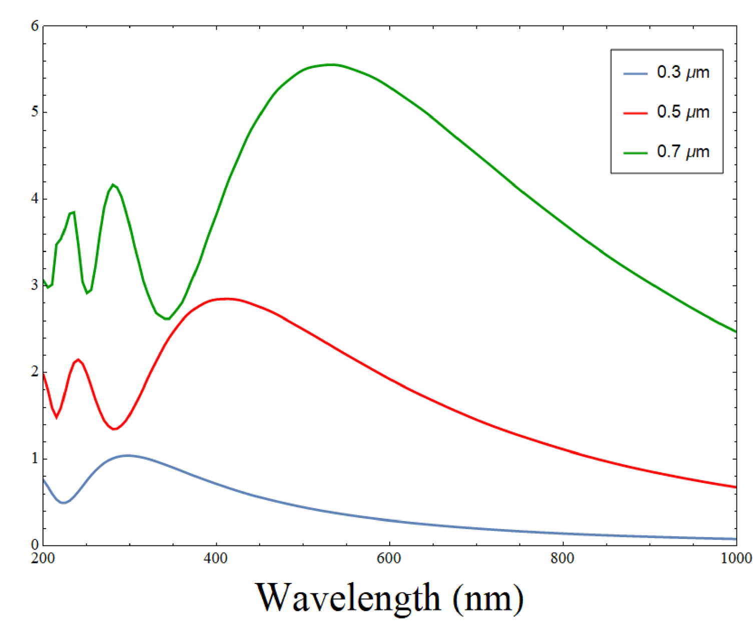


The presence of absorption in a material causes complex behavior of the refractive index

Particle Size Distribution

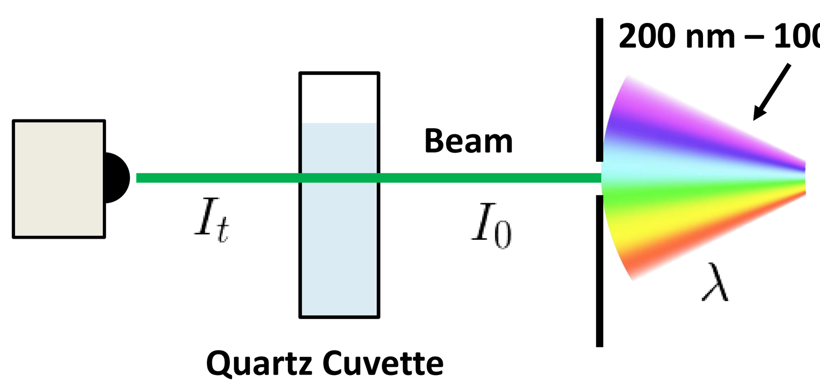
The amount of scattering depends on the size of the particle.

- For a suspension of particles, our simulation weights the scattering contributions assuming the particle sizes follow a bi-modal distribution (to account for particle aggregation)



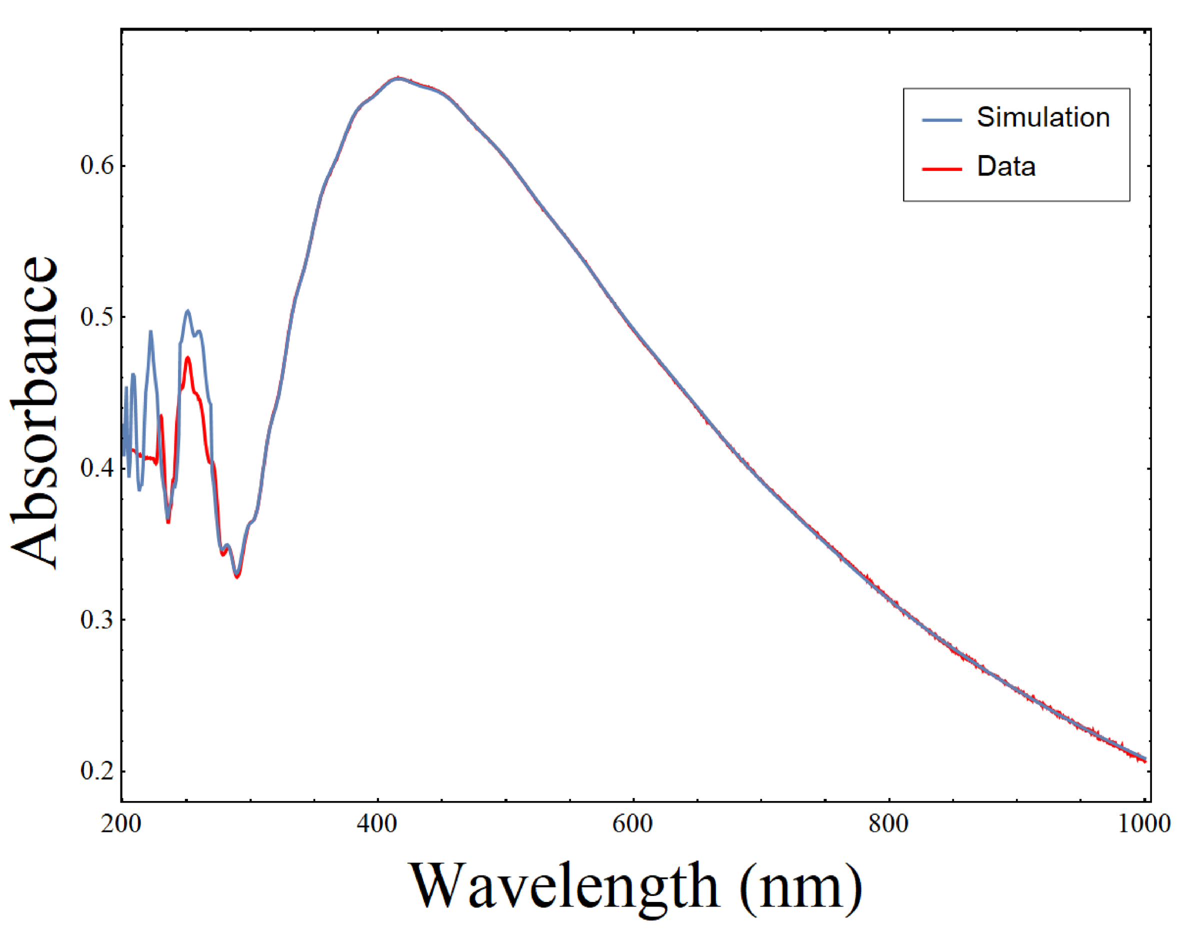
Theoretical scattering spectra for three nominal particle radii

Data Collection



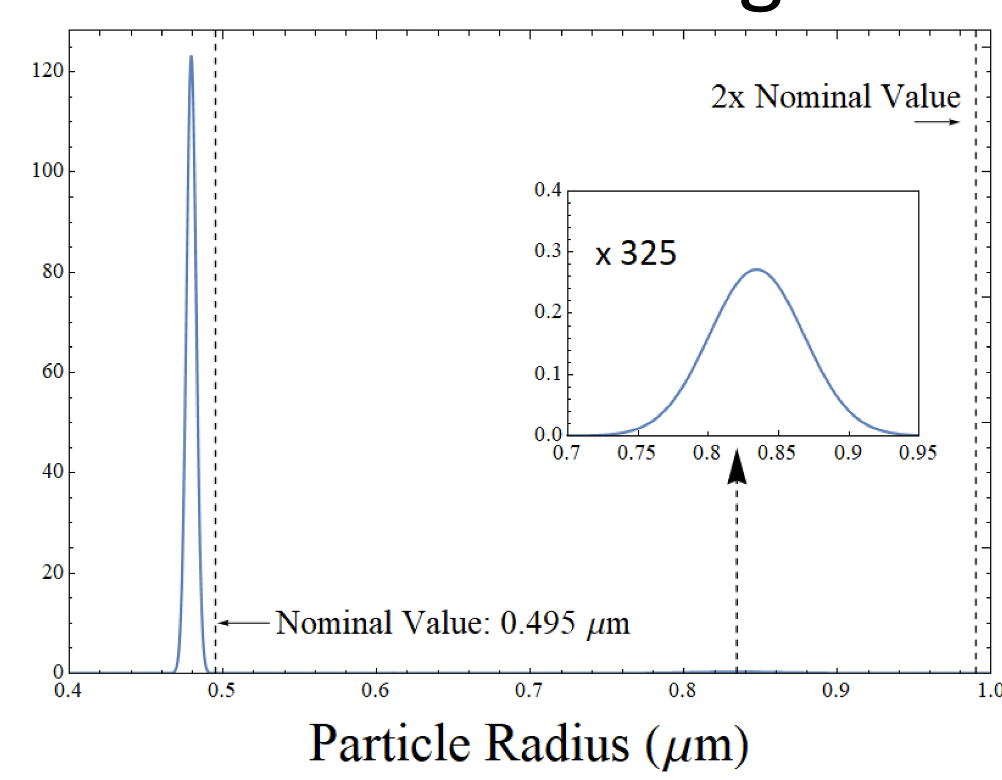
- Extinction spectra are measured from 200 nm to 1000 nm using a Cary 50 UV-Vis Spectrophotometer
- Three samples of beads with radii of 0.495, 0.5125, and 0.5 microns
- The former two samples were purchased already in a water solution
- The latter sample was prepared using dry form beads sonicated into a water/TWEEN 20 surfactant solution

Fit Results



The best fit simulation and the data for the 0.495 micron data set. Similar results were obtained for the other data sets. The fit is nearly perfect from 300 nm – 1000 nm, but deviates below 265 nm when the extinction spectrum becomes a complicated function due absorption/anomalous dispersion.

Particle Sizing

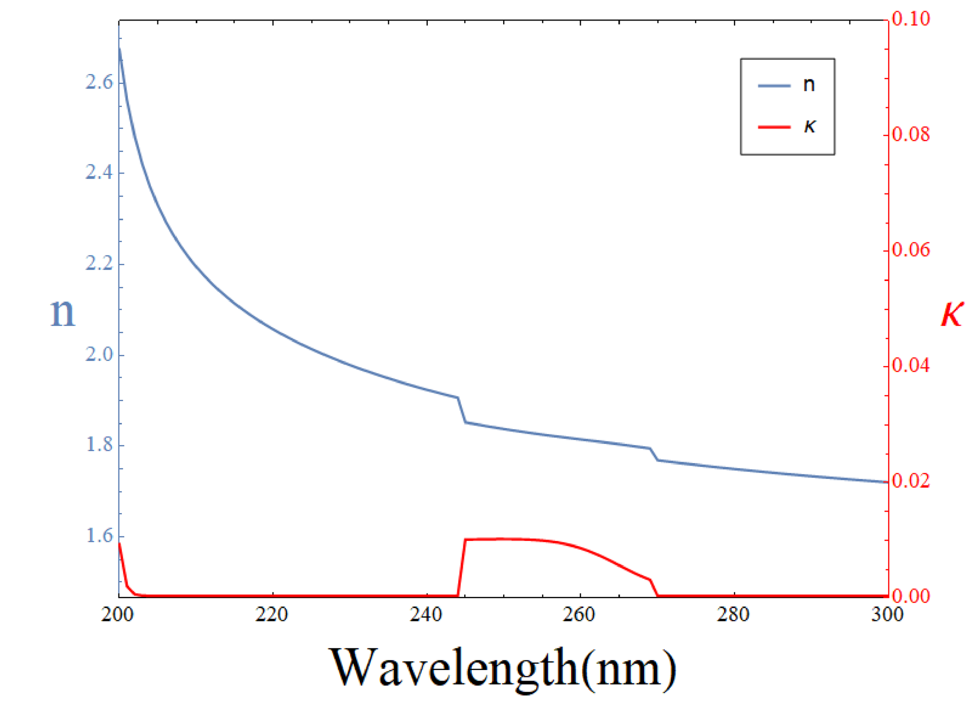


The particle size distribution for the 0.495 micron data set. A small amount of aggregation was detected.

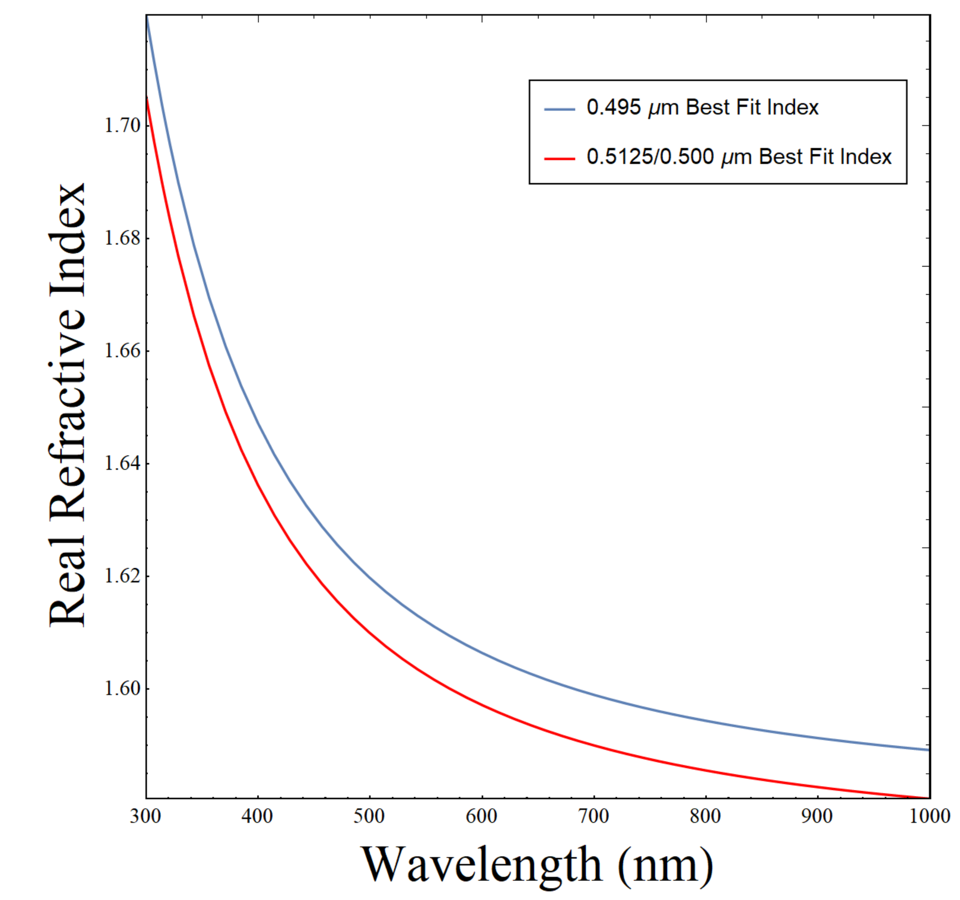
Nominal Radius (μm)	Best Fit Radius (μm)
0.495 ± 0.030	0.4792 ± 0.0032
0.513 ± 0.010	0.5076 ± 0.0033
0.500	0.5099 ± 0.0032

Table. 1. The particle size results for the three data sets

Refractive Index Results



The optical parameters extracted from the simulation are displayed from 200 nm to 300 nm. Our fit suggests that polystyrene has an "absorption shelf" ranging from about 245 nm to 265 nm.



From 300 nm onward, the anomalous dispersion can be neglected, and the index is well described by a Cauchy equation. We find that the refractive index of the 0.495 micron sample is slightly different than the other two.

$$n_{0.495} = 1.58052 + \frac{0.008243}{\lambda^2} + \frac{0.0003856}{\lambda^4}$$

$$n_{0.5125} = 1.57214 + \frac{0.008009}{\lambda^2} + \frac{0.0003562}{\lambda^4}$$

Conclusion

- The refractive index of polystyrene beads can be extracted well from 300 nm – 1000 nm
- We obtain tabulated values for the absorption and anomalous dispersion of polystyrene beads below 300 nm
- Future work will focus on improving agreement between the fit and data below 300 nm