pyBCabsorption

Release 0.1

P. Beeler

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Documentation is always under development, but mostly complete. A manuscript communicating the development of the morphology retrival was published by Atmospheric Chemistry and Physics, and is available here.

NOTE TO USERS: When using pyBCabsorption, pay close attention to the units of the your inputs. Wavelength and particle diameters are always in nanometers, mass absorption cross-sections are in m^2/g. If you use other units, your outputs may not make sense.

CHAPTER

ONE

INSTALL PYBCABS

The current version is 0.0.1. You can install pyBCabs from The Python Package Index (PyPI) with

```
$ pip install pyBCabs==0.0.1
```

or from GitHub. Clone the repository and then run

```
$ python setup.py install
```

CHAPTER

TWO

REVISION HISTORY

- 0.0.1 (30 December, 2022)
  - Initial release.

CHAPTER

THREE

AUTHOR CONTACT INFORMATION

pyBCabs was written by Payton Beeler.

Email: beelerpayton@wustl.edu

3.1 Functions for Internally Mixed Black Carbon Aggregates

3.1.1 Theory

This package computes the core phase shift parameter (ρ_{BC}) to infer the morphology of fractal black carbon aggregates using the particle mass-equivalent diameter (d_p), mass absorption cross-section (MAC_{BC}), and mixing state (M_{tot}/M_{BC}). It should be noted that in this package, MAC_{BC} is defined as the absorption cross-section per unit mass of black carbon. First, ρ_{BC} is constrained by determining whether the measured mass absorption cross-section ($MAC_{BC,meas}$) is significantly less than that given by:

$$MAC_{BC,pred} = MAC_0 \left(\frac{\lambda}{\lambda_0}\right)^{-AAE} \left[1 + \frac{AC^{-B}\Gamma(B+1,C)}{C} - \frac{A\left(\frac{M_{tot}}{M_{BC}}\right)^{B}\left(\frac{M_{tot}}{M_{BC}}\right)^{-B}\Gamma\left(B+1,C\frac{M_{tot}}{M_{BC}}\right)}{C}\right].$$

- $A = -1.189 \pm 0.029$
- $B = -0.674 \pm 0.006$
- $C = 0.043 \pm 0.0007$
- $MAC_0 = 6.819 \pm 0.131$
- $AAE = 1.231 \pm 0.005$

If $MAC_{BC,meas}$ is within 10% of $MAC_{BC,pred}$, then ρ_{BC} can be constrained to $0 < \rho_{BC} < 1$, but cannot be exactly calculated. If $MAC_{BC,meas}$ is less than 90% of $MAC_{BC,pred}$, then ρ_{BC} is calculated by solving:

$$MAC_{BC,meas} = MAC_0 \left(\frac{\lambda}{\lambda_0}\right)^{-AAE} \left[\frac{D}{E+1}\left(\rho_{BC}^{1-E} - 1\right) + \frac{D}{1-2E}\left(\rho_{BC}^{1-2E} - 1\right)\right] + MAC_{BC,pred}.$$

Where D and E are sigmoid functions, given by:

$$X = x_1 + \frac{x_2 - x_1}{1+\exp[x_3(\rho_{BC} - x_4)]}.$$

Here X represents D or E, and $x_{[1,2,3,4]}$ represents $d_{[1,2,3,4]}$ or $e_{[1,2,3,4]}$.

- $d_1 = 5.679 \pm 0.027$
- $d_2 = 1.066 \pm 0.058$
- $d_3 = 0.264 \pm 0.010$
- $d_4 = 11.421 \pm 0.137$

- $e_1 = 2.440 \pm 0.017$
- $e_2 = 0.593 \pm 0.024$
- $e_3 = 0.418 \pm 0.020$
- $e_4 = 10.106 \pm 0.131$

Details on the derivation of the above equations are available here.

The morphology of of the measured black carbon aggregates can be determined by comparing the calculated ρ_{BC} to three cases. The first case is that of freshly emitted black carbon, which has fractal dimension (D_f) of 1.8. The second case is black carbon which has partially collapsed, and has D_f of 2.5. The final case is black carbon which has fully collapsed (but not sintered), and has D_f of 3.0.

The core phase shift parameter of black carbon aggregates with morphologies outlined above is found by first determining their radius of gyration R_g, given by:

$$R_g = a \left(\frac{m_p}{m_1 k_f}\right)^{\frac{1}{D_f}},$$

where a is the monomer radius, k_f is the fractal prefactor (fixed at 1.2), m_p is the black carbon mass, and m_1 is the mass of a BC monomer. Both the BC mass and the monomer mass are determined assuming BC density of 1.8 g/cm^3. Next, the monomer packing fraction (ϕ) is found using:

$$\phi = k_f \left(\frac{D_f+2}{D_f}\right)^{-\frac{3}{2}} \left(\frac{a}{R_g}\right)^{3-D_f}.$$

Finally, ρ_{BC} is given by:

$$\rho_{BC} = \frac{4\pi R_g}{\lambda} |m_{eff} - 1|,$$

where m_{eff} is given by:

$$\phi \left(\frac{m^2-1}{m^2+2}\right) = \left(\frac{m_{eff}^2-1}{m_{eff}^2+2}\right).$$

Here, m is the refractive index of black carbon, $1.95 + 0.79i$. The core phase shift parameter and mass of the measured black carbon aggregates is then compared to the three cases described above, allowing for inference of particle morphology.

In a similar manner, users can supply the morphology, mixing state, and particle diameter, and the mass absorption cross-section can be calculated based on the core phase shift parameter.

3.1.2 Inverse function for single particle

abs2shape_SP(*diameter*, *coating*, *absorption*, *wavelength*[, *k_coat=0.0*, *abs_error=0.0*, *mode='MtotMbc'*, *r_monomer=20*, *asDict=True*, *ReturnPlot=True*, *PlotPoint=True*])

Black carbon mass-equivalent diameter, coating amount, and MAC_{BC} are input and morpholgy is inferred using the procedure outlined above. The particle mass is used to infer the number of monomers, assuming the density of black carbon is 1.8 g/cm^3.

Parameters

diameter
[float] Black carbon mass-equivalent diameter with units of nm.

coating:
Coating amount with units matching that of the optional 'mode' input. Default is ratio of total particle mass to black carbon mass.

absorption:
MAC_{BC} with units of m^2/g.

wavelength
[float] The wavelength of incident light, in nanometers.

k_coat
[float] Imaginary part of coating refractive index.

abs_error
[float, optional] Error associated with measurement of MAC_{BC}, in m^2/g.

mode
[string, optional]

- 'Mtot_Mbc' : ratio of total particle mass to black carbon mass.
- 'Rbc' : ratio of coating mass to black carbon mass.
- 'OC:EC' : ratio of organic carbon mass to black carbon mass.
- 'percent_BC' : percentage of total particle mass which is attributed to black carbon.

r_monomer
[float, optional] Radius of monomers, in nanometers.

asDict
[bool, optional] If true, returns dict of output variables.

ReturnPlot
[bool, optional] If true, returns figure and axes with morphology retrival plot.

PlotPoint
[bool, optional] If true, shows measured particle on morphology retrival plot.

Returns

fig, ax
[figure, axes] Figure and axes with morphology retrival plot. If PlotPoint==True, then particle is shown on morphology retrieval plot.

mass
[float] Mass of particle, in fg.

rho_lower
[float] Lower limit of core phase shift parameter, based on average MAC_{BC} and MAC_{BC} errors.

rho_avg
[float] Average core phase shift parameter, based on average MAC_{BC}.

rho_upper
[float] Upper limit of core phase shift parameter, based on average MAC_{BC} and MAC_{BC} errors.

3.1.3 Forward function for single particle

shape2abs_SP(*dp*, *coating*, *collapse*, *wavelength*[, *k_coat=0.0*, *mode='MtotMbc'*, *r_monomer=20*, *asDict=True*])

Black carbon mass-equivalent diameter, coating amount, and morphology are input and MAC_{BC} is calculated using the procedure outlined above.

Parameters

dp
[float] Black carbon mass-equivalent diameter with units of nm.

coating
[float] Coating amount with units matching that of the optional 'mode' input. Default is ratio of total particle mass to black carbon mass.

collapse
[string]

- 'fresh' : black carbon morphology matches fresh soot with fractal dimension of 1.8.
- 'partial' : black carbon core has partially collapsed, fractal dimension of 2.5.
- 'full' : black carbon core has fully collapsed, fractal dimension of 3.0.

wavelength
[float] The wavelength of incident light, in nanometers.

k_coat
[float]

- Imaginary part of coating refractive index.

mode
[string, optional]

- 'Mtot_Mbc' : ratio of total particle mass to black carbon mass
- 'Rbc' : ratio of coating mass to black carbon mass
- 'OC:EC' : ratio of organic carbon mass to black carbon mass
- 'percent_BC' : percentage of total particle mass which is attributed to black carbon.

r_monomer
[float, optional] Radius of monomers, in nanometers.

asDict
[bool, optional] If true, returns dict of output variables.

Returns

dp
[float] Mass-equivalent diameter of particle in nm.

coating
[float] Amount of coating with same units as input.

MAC
[float] MAC_{BC} with units of m^2/g.

3.1.4 Inverse function for black carbon size distribution

abs2shape_SD(*dpg*, *sigma_g*, *coating*, *absorption*, *wavelength*[, *k_coat=0.0*, *abs_error=0.0*, *mode='MtotMbc'*, *r_monomer=20*, *asDict=True*, *ReturnPlot=True*])

Black carbon mass-equivalent lognormal size distribution, coating amount, and MAC_{BC} are input and morpholgy is inferred using the procedure outlined above. The particle mass is used to infer the number of monomers, assuming the density of black carbon is 1.8 g/cm^3.

Parameters

dpg
[float] Black carbon geometric mean mass-equivalent diameter of lognormal distribution with units of nm.

sigma_g
[float] Geometric standard deviation of black carbon lognormal size distribution.

coating:
Coating amount with units matching that of the optional 'mode' input. Default is ratio of total particle mass to black carbon mass.

absorption:
MAC_{BC} with units of m^2/g.

wavelength
[float] The wavelength of incident light, in nanometers.

k_coat
[float]

- Imaginary part of coating refractive index.

abs_error
[float, optional]

- Error associated with measurement of MAC_{BC}, in m^2/g.

mode
[string, optional]

- 'Mtot_Mbc' : ratio of total particle mass to black carbon mass.
- 'Rbc' : ratio of coating mass to black carbon mass.
- 'OC:EC' : ratio of organic carbon mass to black carbon mass.
- 'percent_BC' : percentage of total particle mass which is attributed to black carbon.

r_monomer
[float, optional] Radius of monomers, in nanometers.

asDict
[bool, optional] If true, returns dict of output variables.

ReturnPlot
[bool, optional] If true, returns figure and axes with morphology retrival plot.

Returns

fig, ax
[figure, axes] If ReturnPlot==True, figure and axes with morphology retrival plot.

lower_mass
[float] Average-standard deviation of mass of particles, in fg.

avg_mass
[float] Average mass of particles, in fg.

upper_mass
[float] Average+standard deviation of mass of particles, in fg.

rho_lower
[float] Lower limit of core phase shift parameter, based on average MAC_{BC} and MAC_{BC} errors.

rho_avg
[float] Average core phase shift parameter, based on average MAC_{BC}.

rho_upper
[float] Upper limit of core phase shift parameter, based on average MAC_{BC} and MAC_{BC} errors.

3.1.5 Forward function for black carbon size distribution

shape2abs_SD(*dpg*, *sigma_g*, *coating_avg*, *coating_stdev*, *collapse*, *wavelength*[, *k_coat=0.00*, *mode='MtotMbc'*, *r_monomer=20*, *DataPoints=False*, *ShowPlots=True*])

Black carbon mass-equivalent lognormal size distribution, coating distribution, and morphology are input and distribution of MAC_{BC} is calculated. Black carbon mass-equivalent diameter and coating amount are randomly sampled per the input distributions, and MAC_{BC} is calculated using the procedure outlined above.

Parameters

dpg
[float] Black carbon geometric mean mass-equivalent diameter of lognormal distribution with units of nm.

sigma_g
[float] Geometric standard deviation of black carbon lognormal size distribution

coating_avg
[float] Average value of coating amount, assuming a Gaussian normal distribution. Units should match that of the optional 'mode' input, default is ratio of total particle mass to black carbon mass.

coating_stdev
[float] Stabdard deviation of coating amount, assuming a Gaussian normal distribution.

collapse
[string]

- 'fresh' : black carbon morphology matches fresh soot with fractal dimension of 1.8.
- 'partial' : black carbon core has partially collapsed, fractal dimension of 2.5.
- 'full' : black carbon core has fully collapsed, fractal dimension of 3.0.

wavelength
[float] The wavelength of incident light, in nanometers.

k_coat
[float]

- Imaginary part of coating refractive index.

mode
[string, optional]

- 'Mtot_Mbc' : ratio of total particle mass to black carbon mass
- 'Rbc' : ratio of coating mass to black carbon mass
- 'OC:EC' : ratio of organic carbon mass to black carbon mass
- 'percent_BC' : percentage of total particle mass which is attributed to black carbon.

r_monomer
[float, optional] Radius of monomers, in nanometers.

DataPoints
[bool, optional] If true, returns dict of output variables.

ShowPlots
[bool, optional] If true, shows histograms of input parameters and calculated MAC_{BC}.

Returns

dp
[float]

- If DataPoints==True, mass-equivalent black carbon diameters used in calculations, in nm.
- If DataPoints==False, average and standard deviation of mass-equivalent black carbon diameters used in calculations, in nm.

coating
[float]

- If DataPoints==True, coating amounts used in calculations, with units matching those of 'mode' option.
- If DataPoints==False, average and standard deviation of coating amounts used in calculations, with units matching those of 'mode' option.

MAC
[float]

- If DataPoints==True, calculated MAC_{BC} values, in m^2/g.
- If DataPoints==False, average and standard deviation of calculated MAC_{BC} values, in m^2/g.

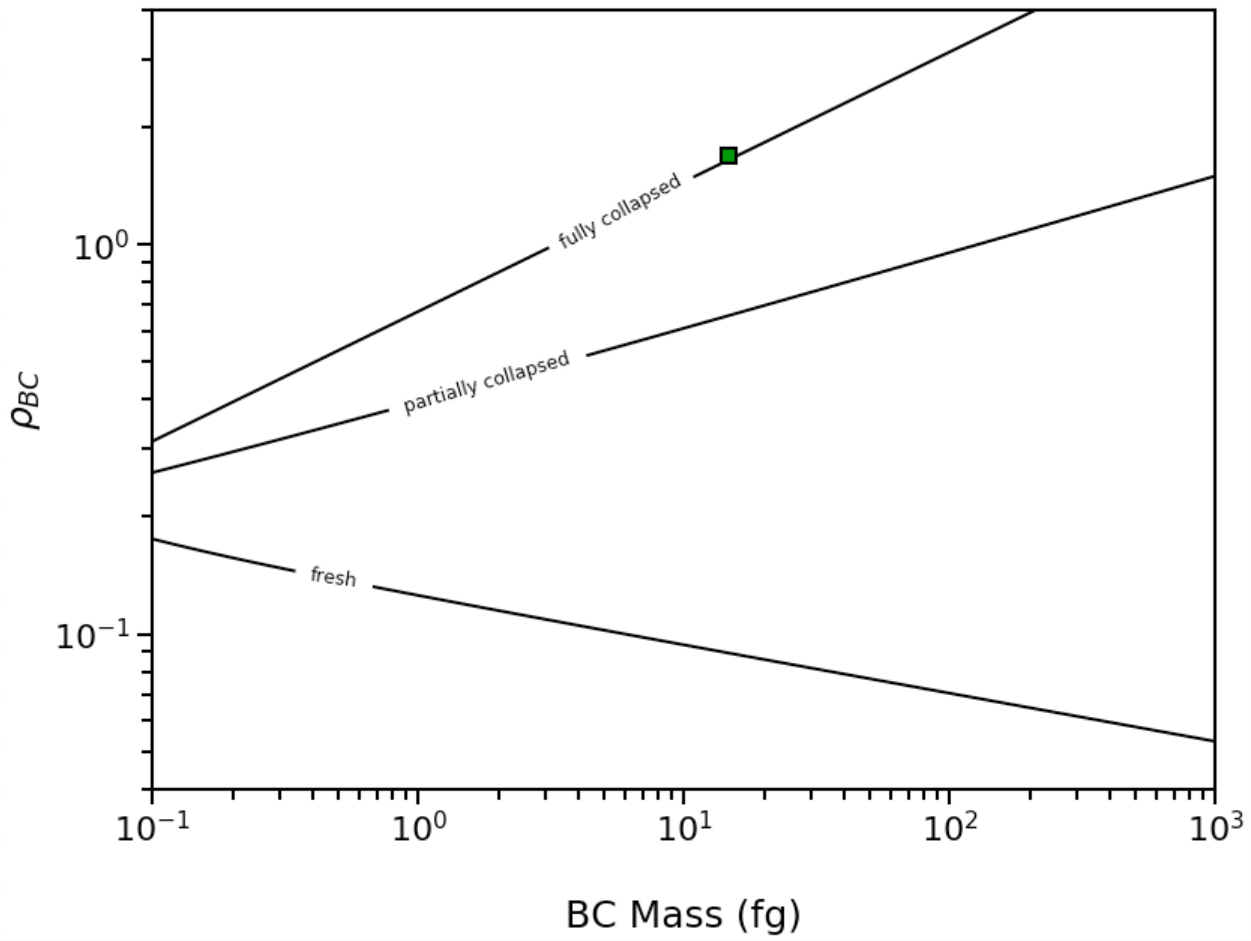
3.2 Example Scripts

3.2.1 Morphology of of a Single Black Carbon Particle

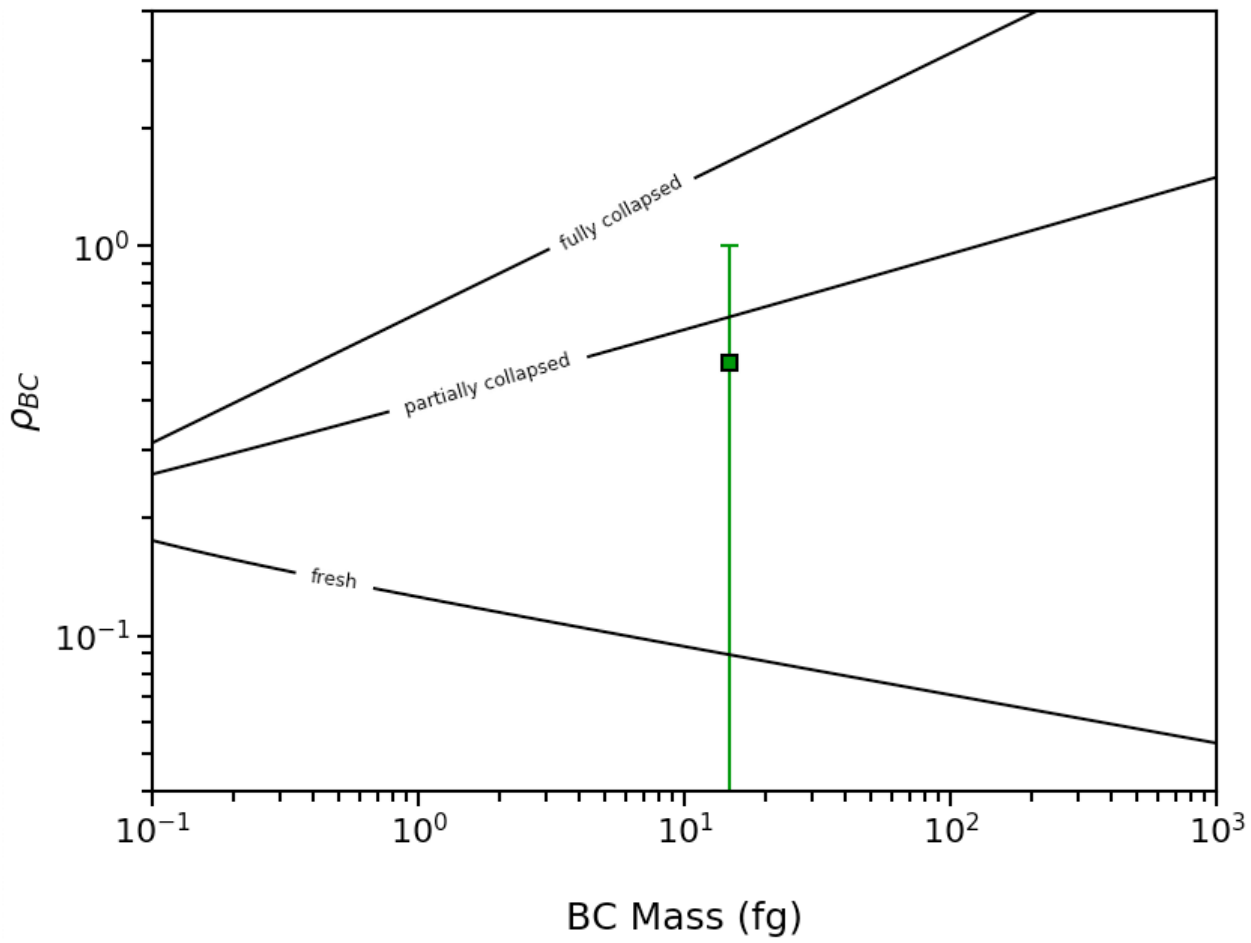
To infer the morphology of a single BC particle, use the *abs2shape_SP()* function. This example shows a particle with mass-equivalent diameter of 250nm, M_{tot}/M_{BC} of 10, and MAC_{BC} of 12.5 m^2/g measured at 532 nm, coated with non-absorbing material.

```
>>> import pyBCabs.retrival as pyBCabs
>>> pyBCabs.abs2shape_SP(250, 10, 12.5, 532, k_coat=0.00, ReturnPlot=False,␣
↪PlotPoint=True)
{'mass': 14.726215563702151,
'rho_lower': 1.6958737655127754,
'rho': 1.6958737655127754,
'rho_upper': 1.6958737655127754}
```

This particle has $\rho_{BC} > 1$, and generates this morphology plot:



If the measured MAC_{BC} were 15 m^2/g, then $0 < \rho_{BC} < 1$, and this morphology plot will be generated:



If you wish to plot multiple particle-resolved measurements, this can also be done using the *abs2shape_SP()* function.

```
wl=532 #wavelength
dp=np.logspace(np.log10(150),np.log10(250),10) #example BC mass-equivalent diameter measurements
M=10 #coating amount
p_avg=np.zeros(len(dp))
lower=np.zeros(len(dp))
upper=np.zeros(len(dp))
mass=np.zeros(len(dp))

fig, ax, result = pyBCabs.abs2shape_SP(1, M, 6.4, wl, k_coat=0.0, abs_error=1.0, ReturnPlot=True, PlotPoint=False)

for i in range(0,len(dp)):

    MAC=np.random.normal(0.8,0.1)*15
    result=pyBCabs.abs2shape_SP(dp[i], M, MAC, wl, k_coat=0.0, abs_error=1.0, ReturnPlot=False, PlotPoint=False)
    mass[i]=result['mass']
    p_avg[i]=result['rho']
    lower[i]=result['rho']-result['rho_lower']
    upper[i]=result['rho_upper']-result['rho']
```

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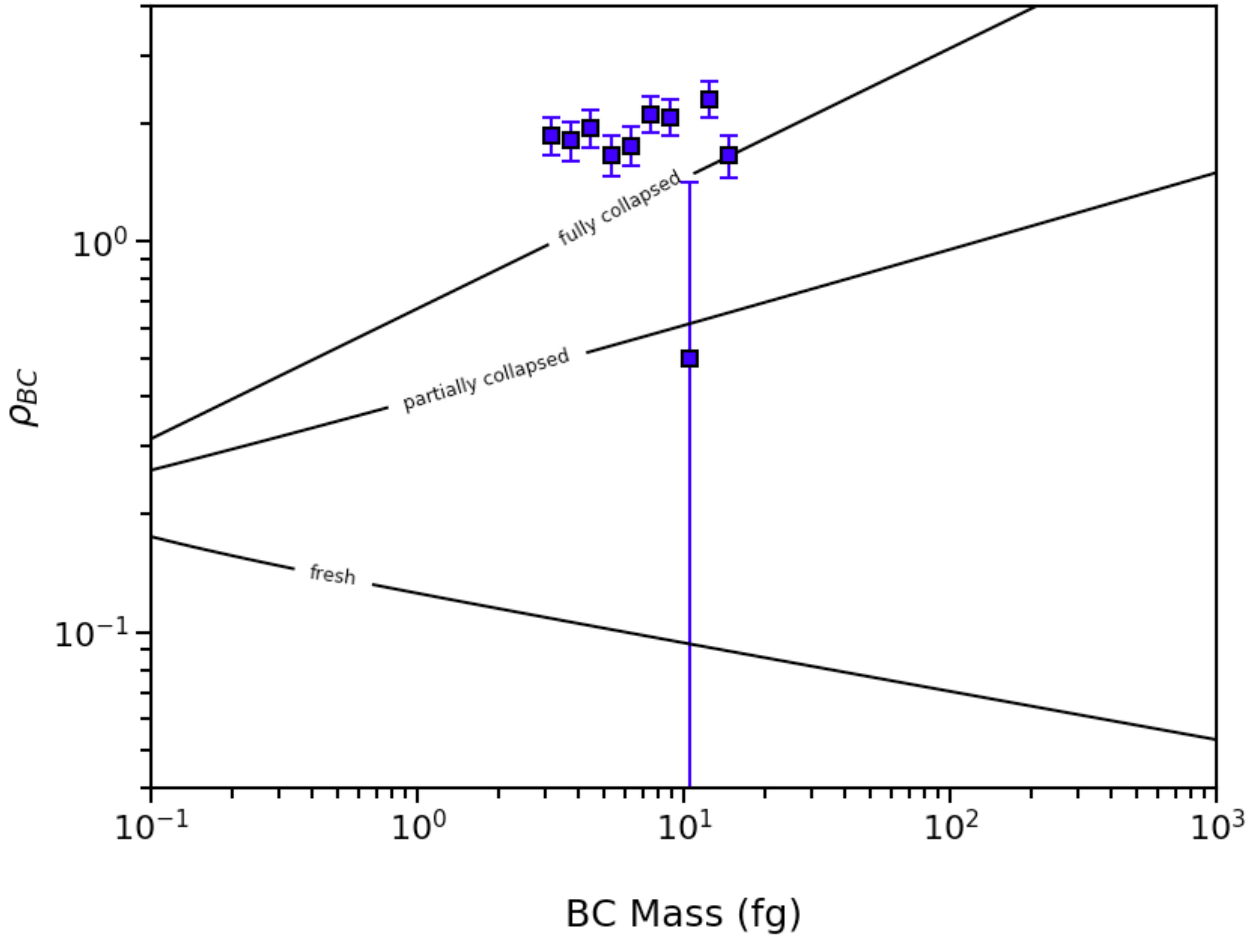
```
errors=np.row_stack((lower,upper))
ax.errorbar(mass, p_avg, yerr=errors, markersize=7, fmt = 's', mfc='b', mec = 'k',␣
↪capsize=4, ecolor = 'b', elinewidth=1.5, mew=1.5)
plt.show()
```

The above code will generate a plot similar to this:



3.2.2 Absorption of of a Single Black Carbon Particle

To calculate MAC_{BC} of a single particle, use the *shape2abs_SP()* function. This example shows a partially collapsed BC particle with mass-equivalent diameter of 250nm and M_{tot}/M_{BC} of 10, calculated at 532 nm, with non-absorbing coating.

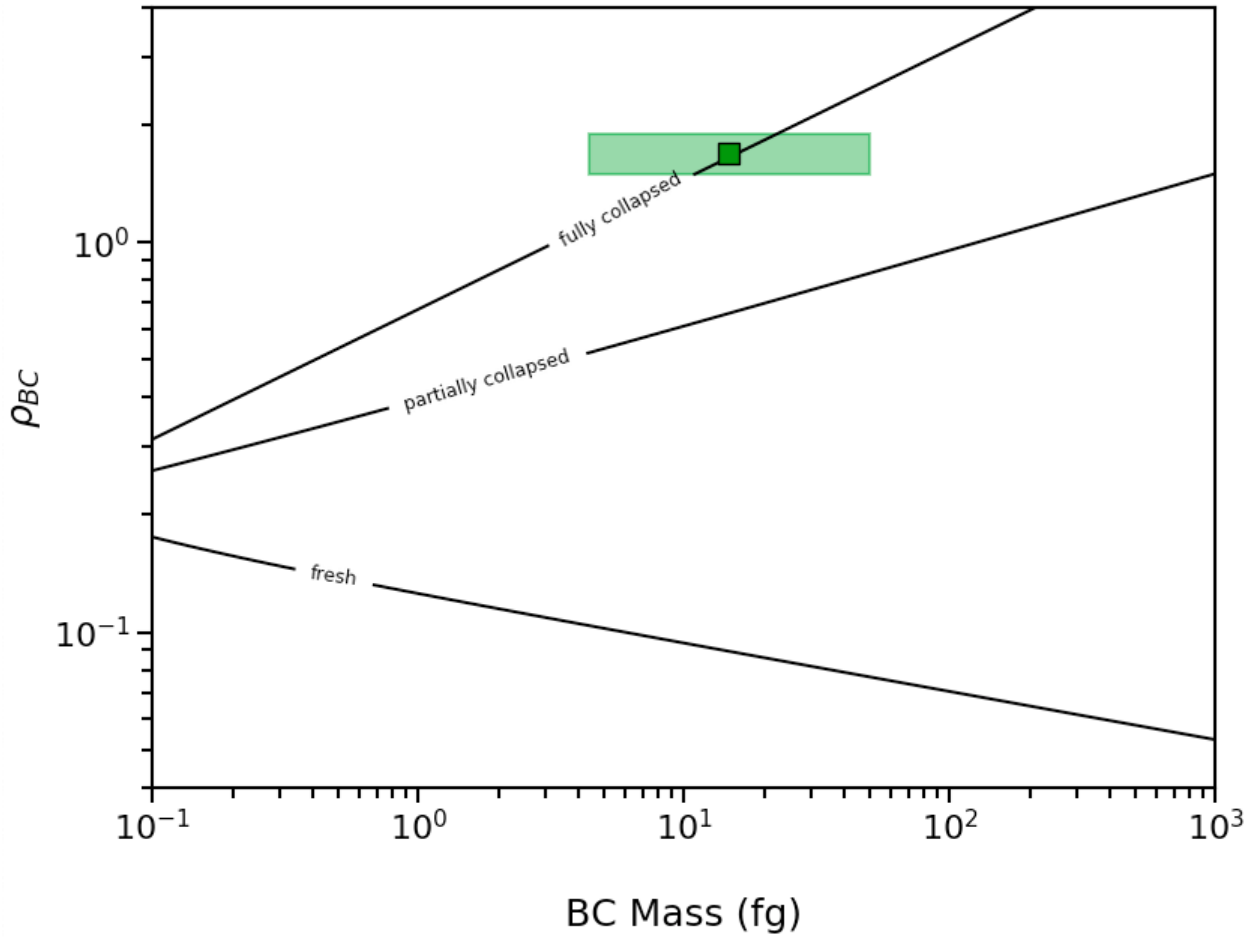
```
>>> import pyBCabs.retrival as pyBCabs
>>> pyBCabs.shape2abs_SP(250, 10, 'partial', 532, k_coat=0.00, mode='MtotMbc', r_
↪monomer=20, asDict=True)
{'dp': 250,
'coating': 10,
'MAC': 15.270921290660958}
```

3.2.3 Morphology of Black Carbon Size Distribution

To infer the morphology of a lognormal size distribution of black carbon particles, use the *abs2shape_SD()* function. This example shows a distribution of black carbon with geometric mean mass-equivalent diameter of 250nm, geometric standard deviation of 1.5, M_{tot}/M_{BC} of 10, and MAC_{BC} of 12.5 m^2/g measured at 532 nm, with non-absorbing coating.

```
>>> import pyBCabs.retrival as pyBCabs
>>> pyBCabs.abs2shape_SD(250, 1.5, 10, 12.5, 532, k_coat=0.0, abs_error=1.0,␣
↪ReturnPlot=True)
<Figure size 832x624 with 1 Axes>,
<matplotlib.axes._subplots.AxesSubplot object at 0x119e22e80>,
{'min_mass': 4.363323129985816,
'avg_mass': 14.726215563702134,
'max_mass': 49.70097752749473,
'rho_lower': 1.4961402652726399,
'rho': 1.6958737655127754,
'rho_upper': 1.9011038545429513}
 >>> plt.show()
```

The above code will generate the following plot:

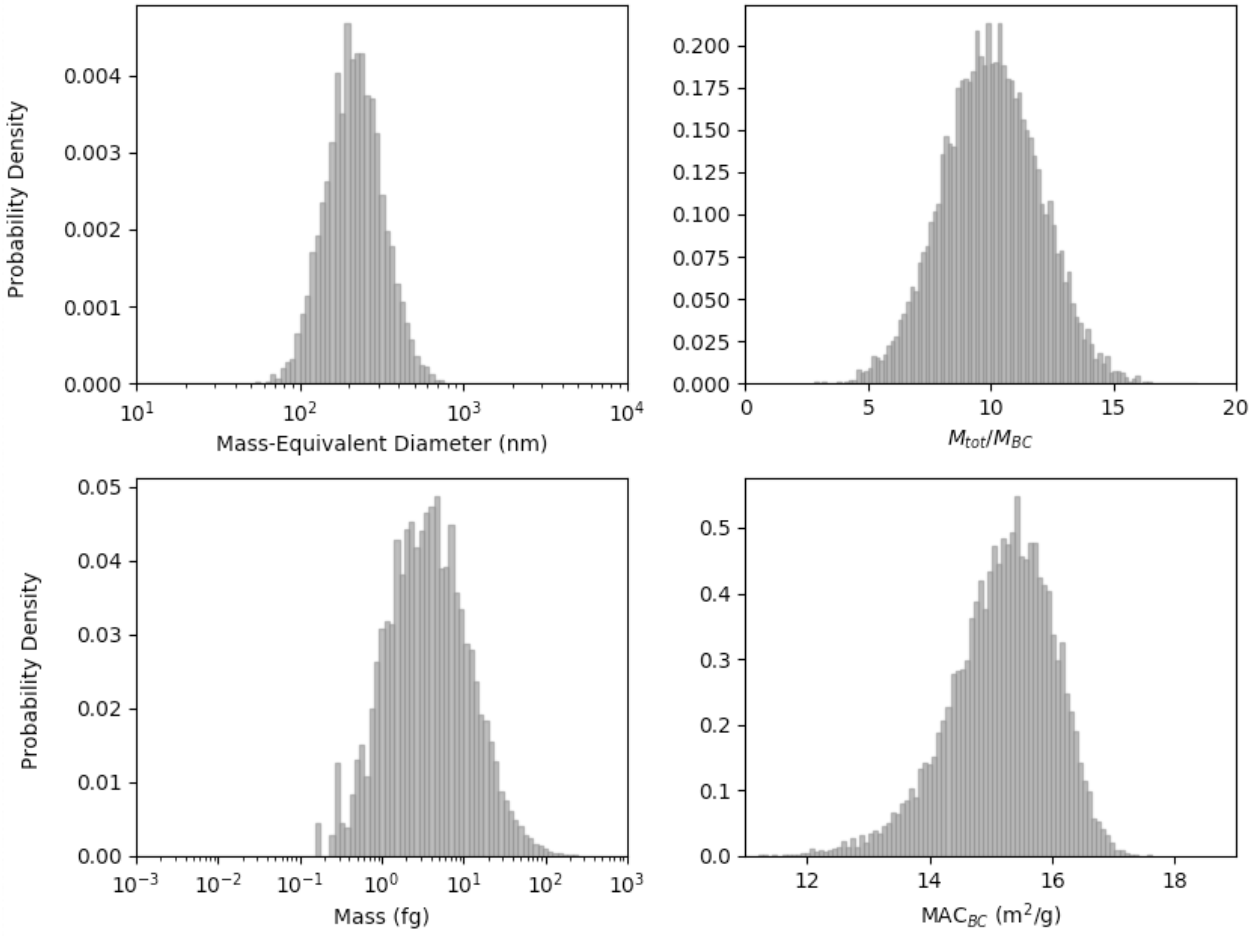


3.2.4 Absorption of of a Black Carbon Size Distribution

To calculate MAC_{BC} of a lognormal black carbon size distribution, use the *shape2abs_SD()* function. This example shows a partially collapsed black carbon size distribution with geometric mean mass-equivalent diameter of 250nm, geometric standard deviation of 1.5, and M_{tot}/M_{BC} of 10 (with standard deviation of 2), calculated at 532 nm, with non-absorbing coating.

```
>>> import pyBCabs.retrival as pyBCabs
>>> pyBCabs.shape2abs_SD(250, 1.5, 10, 2, 'partial', 532, k_coat=0.00, mode='MtotMbc', r_
↪monomer=20, DataPoints=False, ShowPlots=True)
{'dp_avg': 271.1435259574555,
'dp_stdev': 115.42341830345885,
'coating_avg': 9.989282292286155,
'coating_stdev': 1.9791873855346263,
'MAC_avg': 15.165034433016245,
'MAC_std': 0.8543285503019649}
```

The following plot is also generated:



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