IMPLEMENTING THE AGGREGATE OPTICS MODEL

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The coated sphere code used in this model was developed by Xiaodong Zhang (1998) funded by the U.S. Office of Naval Research and the Canadian Natural Sciences and Engineering Research Council
Zhang, X., Lewis, M., and Johnson, B. (1998). Influence of bubbles on scattering of light in the ocean. Appl. Opt. 37, 6525–6536.

NOTATION

Symbol	Description	
D_A	Characteristic length scale of aggregate (typically diameter of sphere enclosing aggregate, or length of longest side of aggregate)	
D_M	Diameter of equivalent-mass (or solid volume) sphere	
D_0	Diameter of monomer	
d_n	Fractal dimension of aggregate in n dimensions	
N	Number of monomer particles in aggregate	$N = \left(\frac{D_A}{D_0}\right)^{d_3}$
M_0	Mass of monomer particle	
M_A	Mass of aggregate	$M_A = M_0\left(\frac{D_A}{D_0}\right)^{d_3}$
G_A	Cross-sectional area presented by sphere enclosing aggregate	
G_M	Cross-sectional area presented by equivalent-mass sphere	
V_A	Volume of sphere enclosing aggregate	$V_A = \frac{\pi}{6}D_A^3$
V_M	Solid volume of aggregate	
V_0	Volume of monomer	$V_0 = \frac{\pi}{6}D_0^3$
F	Solid fraction of aggregate	$F = V_M/V_A$
P	Porosity of aggregate	$P = 1 - F$
d_n	Fractal dimension of aggregate in n dimensions	

SUMMARY OF LATIMER'S MODEL

From Latimer (1985):

> "Our approximate method of predicting its scattering properties represents the aggregate by a model of the same gross volume and net mass but of a different shape and structure. The method is based on postulates of soft-particle approximations. Two aggregate geometries were used in theoretical predictions: the randomly oriented spheroid and the hollow sphere. The first simulates some of the irregularities of the randomly oriented aspherical aggregate, the second simulates some of its inhomogeneities."
>
> "The volume of the coat of the hollow sphere and its refractive index are set equal to those of the component particles… The volume and refractive index of the core are set equal to those of the spaces between the particles… The gross volume of the homogeneous spheroid is also set equal to the gross volume of the aggregate. Its refractive index is the average value weighted in proportion to the volumes of the component particles and the spaces. For aggregates of three or more particles modeled as prolate spheroids, the axial ratio was taken as 3:1."
>
> "While each model should approximate aggregate scattering, it will also predict singularities peculiar to itself. Hence, as a best theoretical estimate, we use the average prediction for the two different models for comparisons of theoretical predictions with experimental findings."

SPHEROID MODEL

The spheroid model used here transforms a given spheroid geometry into a polydispersion of spheres (Paramonov 1994). Implementation of the spheroid model is based on Shepelevich (2001) and centers around the integral in his equation (18):

$$C_{ext,abs}^{spheroid} = \int_{\alpha}^{\alpha\epsilon} C_{ext,abs}^{sphere}(x) f(x) dx$$

where:

$\alpha = kb$, k is the wavenumber in the surrounding medium, b is the semisize of the axis of revolution;

$\epsilon = a/b$, is the axial ratio; and

$f(x)$ is the power law size distribution describing the polydispersion of spheres.

The power law distribution is designed to have average surface area and volume equal to the surface area and volume of the spheroid.

$$f(x) = \frac{\epsilon^4 \alpha^5}{(\epsilon^2 - 1)x^5} \sqrt{\frac{\epsilon^2 - 1}{\alpha^2 \epsilon^2 - x^2}}$$

For the aggregate model, we consider the characteristic size of the aggregate to be the diameter of the sphere that encloses the aggregate (what Latimer terms the "gross volume") and then determine the size of the spheroid having the same volume, keeping the axial ratio 1:3.

The volume of spheroid is $V_{spheroid} = \frac{4}{3}\pi a^2 b$, and in terms of b and ϵ becomes, $V_{spheroid} = \frac{4}{3}\pi \epsilon^2 b^3$, so we can determine the size of the spheroid in terms of the characteristic size of the aggregate:

$$V_{spheroid} = V_A$$

$$\frac{4}{3}\pi \epsilon^2 b^3 = \frac{\pi}{6} D_A^3$$

$$b = \frac{1}{2} D_A \epsilon^{\frac{2}{3}}$$

Finally, converting to size parameter and wavelength,

$$\alpha = \frac{\pi}{\lambda} D_A \epsilon^{\frac{2}{3}}.$$

Within LatimeterAggregate.m, the spheroid model is realized as:

```
alpha = (pi/lambda)*D_A*epsilon^(2/3);
Cext_spheroid =
quadgk(@(x)Cext_fx(x,alpha,epsilon,m_eff,mp_eff,k),alpha,alpha.*epsilon);
```

With function Cext_fx:

```
function g = Cext_fx(x, alpha, epsilon, m,mp, k)

    % Extinction of sphere according to anomalous diffraction model of VDH
    rho = 2*x*(m-1);
    beta = atan(mp/(m-1));
    Qext = 2-4*exp(-rho*tan(beta)) .* (cos(beta)*sin(rho-
beta)./rho+(cos(beta)./rho).^2 .* cos(rho-2*beta)) ...
        + 4*(cos(beta)./rho).^2 * cos(2*beta);

    % power-law size distribution of equivalent sphere polydispersion
    f_x = (epsilon^4*alpha^5)./((epsilon^2-1)*x.^5) .* sqrt((epsilon^2-
1)./(alpha^2*epsilon^2-x.^2));

    g = (Qext.*pi.*x.^2./k^2) .* f_x;

return
```

Note that the integral is not well-behaved at $x = \alpha\epsilon$, so the QUADGK is used. It may also be necessary to nudge the limits of the integral, for example `alpha*epsilon*1. 00000000001`.

The index of refraction of the spheroid is determined using a simplification of the Gladstone-Dale rule for effective index of refraction of an inhomogeneous mixture (see Jonasz and Fournier 2007 p466):

$m_{eff} = 1 + \sum_j F_j(m_j - 1)$, where F_j and m_j are the volume fraction and complex index of refraction of the j-th component in the mixture. For the aggregate, component 1 is the solid particulate matter and component 2 is seawater, but the refractive index of the solid is given in relative terms, thus $m_2 = 1$, leading to

$$m_{eff} = 1 + F(m - 1).$$

Then real and imaginary parts are:

$$Re\{m_{eff}\} = 1 + F(Re\{m\} - 1)$$

$$Im\{m_{eff}\} = FIm\{m\}$$

HOLLOW SPHERE MODEL

The coated sphere code was developed by X. Zhang (1998). For the optical model of the aggregate, the volume of the coat and core of the particle are set equal to the volume of the component particles and void, respectively; and the indices of refraction for the coat and core are set equal to those of the component solids and interior medium, respectively.

The Zhang coated sphere model requires 4 parameters,

```
%   m = relative refractive index of the (core) particle
%   x = size parameter of the (core) particle, could be a vector
%   m2 = relative refractive index of the coating
%   y = size parameter of the ENTIRE particle (core size + coating thickness),
could be a vector
```

To specify the geometry of the hollow sphere in terms of the aggregate size and structure, the core volume is defined using the characteristic aggregate size and solid fraction:

$$V_{core} = PV_A = (1 - F)V_A = (1 - F)\frac{\pi}{6}D_A^3$$

$$D_{core} = (1 - F)^{\frac{1}{3}}D_A$$

$$x = \frac{\pi}{\lambda}(1 - F)^{\frac{1}{3}}D_A$$

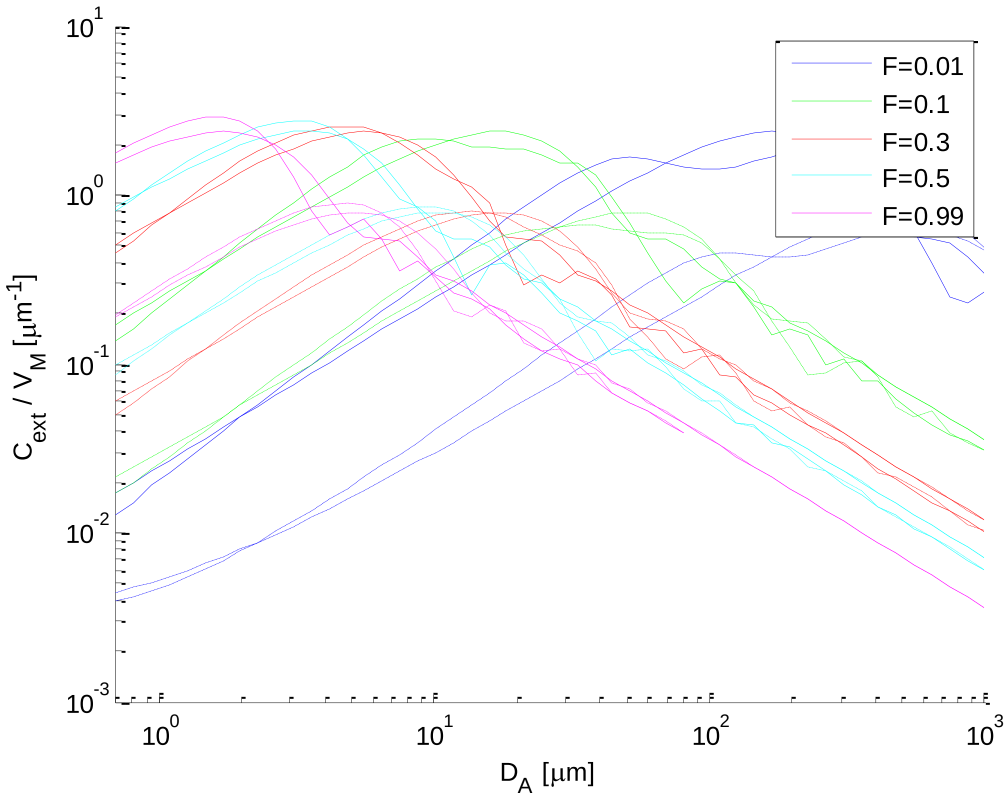
Because the total volume of the hollow sphere must equal the total enclosed volume of the aggregate,

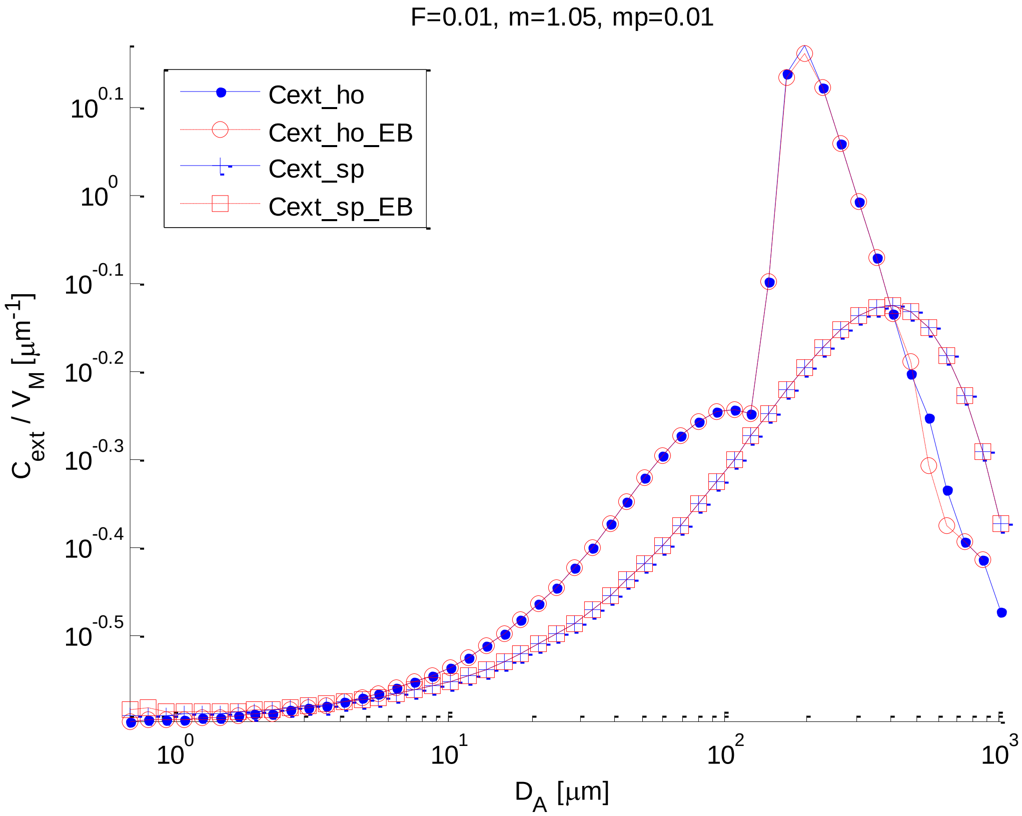
$$D_{core+coat} = D_A$$

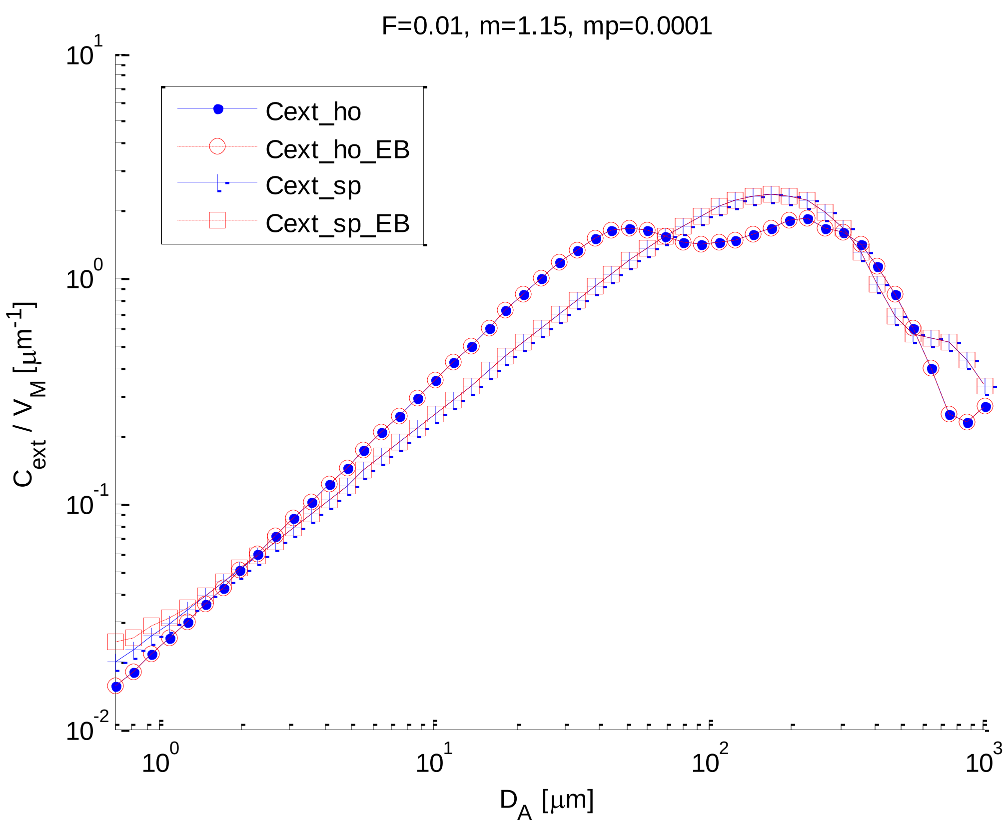
$$y = \frac{\pi}{\lambda}D_A$$

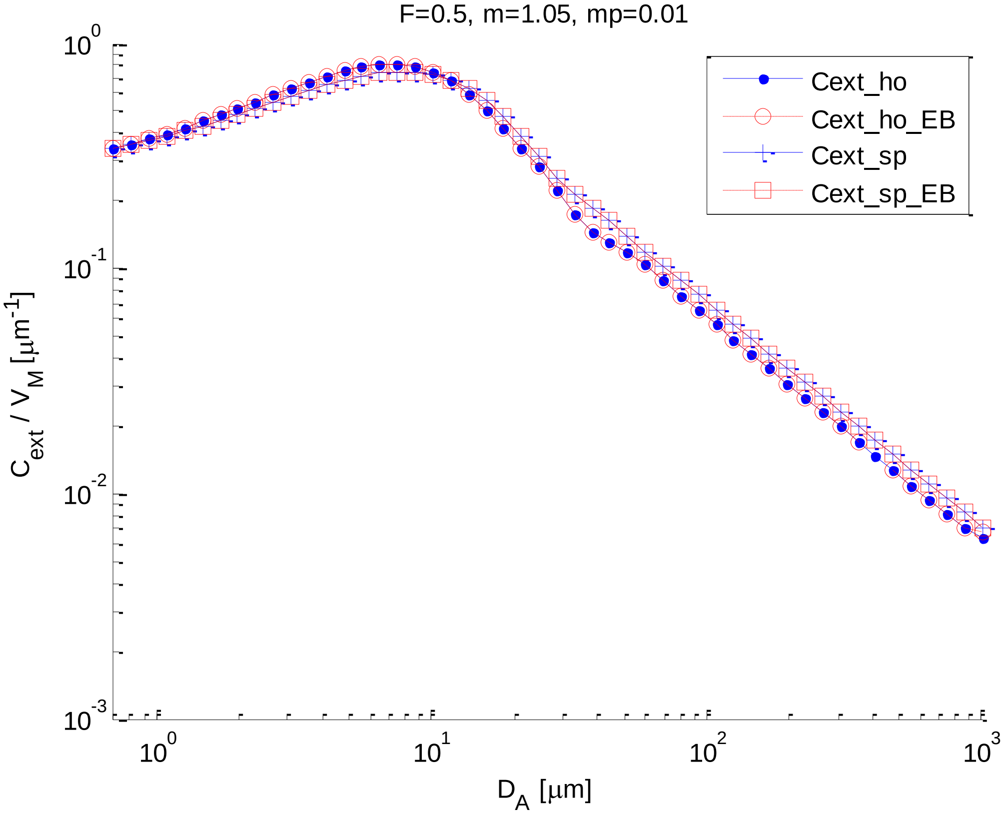
VALIDATION

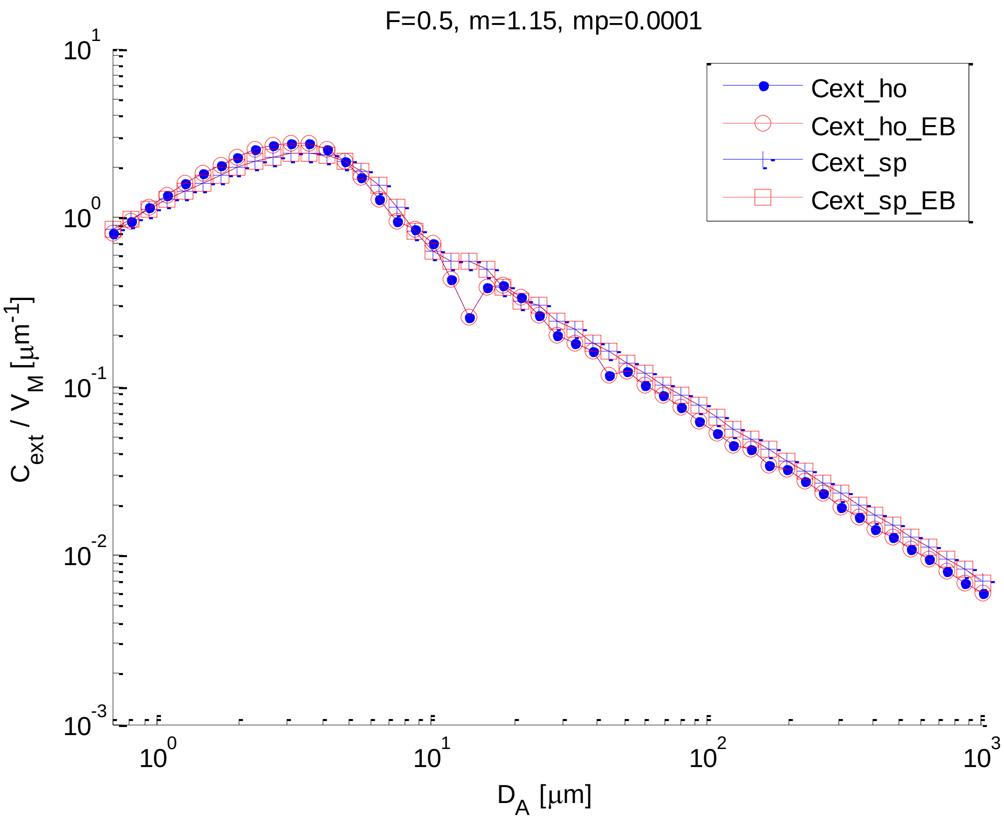
I extracted and encapsulated the calculations in Emmanuel's code (EB_Zhang, EB_Shepelevich) and compared to my own code for 6 cases: F = {0.01, 0.5, 0.9} and m+im$_p$= {0.05+0.01i,0.15+0.0001}. The algorithms in EB_Zhang and EB_Shepelevich are written in terms of the equivalent mass diameter D_M, so a conversion is made within the Test_Aggregate script.

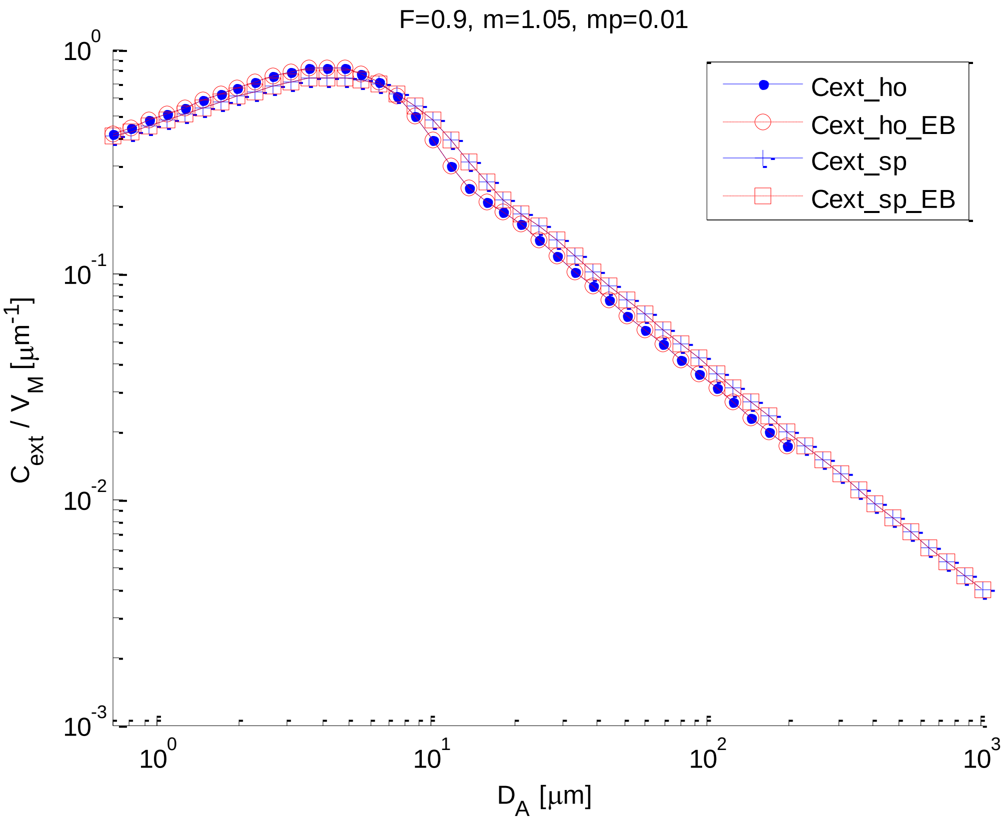


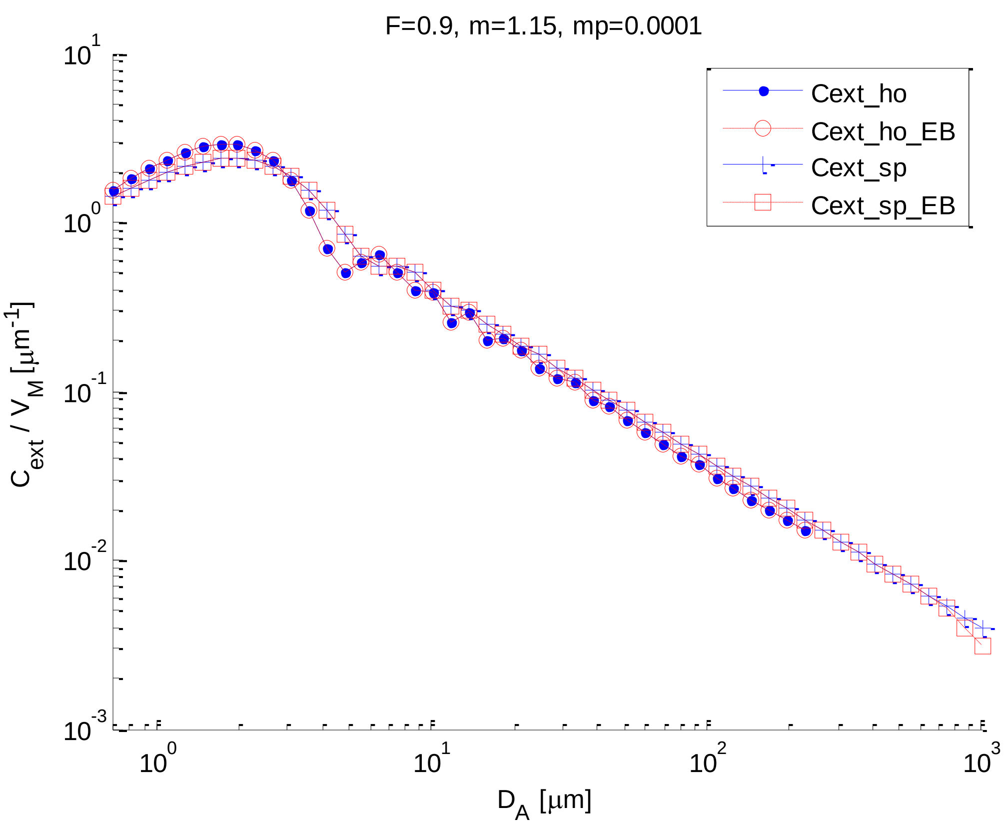

F=0.01, m=1.05, mp=0.01
Cext_ho
Cext_ho_EB
Cext_sp
Cext_sp_EB
$10^{0.1}$
10^{0}
$10^{-0.1}$
$10^{-0.2}$
$10^{-0.3}$
$10^{-0.4}$
$10^{-0.5}$
C_{ext} / V_M [μm^{-1}]
10^{0}
10^{1}
10^{2}
10^{3}
D_A [μm]


F=0.01, m=1.15, mp=0.0001
Cext_ho
Cext_ho_EB
Cext_sp
Cext_sp_EB
10^{1}
10^{0}
10^{-1}
10^{-2}
C_{ext} / V_M [μm^{-1}]
10^{0}
10^{1}
10^{2}
10^{3}
D_A [μm]


F=0.5, m=1.05, mp=0.01
Cext_ho
Cext_ho_EB
Cext_sp
Cext_sp_EB
C_{ext} / V_M [μm^{-1}]
D_A [μm]
10^0
10^{-1}
10^{-2}
10^{-3}
10^0
10^1
10^2
10^3


F=0.5, m=1.15, mp=0.0001
Cext_ho
Cext_ho_EB
Cext_sp
Cext_sp_EB
C_{ext} / V_M [μm^{-1}]
D_A [μm]
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^0
10^1
10^2
10^3


F=0.9, m=1.05, mp=0.01
Cext_ho
Cext_ho_EB
Cext_sp
Cext_sp_EB
C_{ext} / V_M [μm^{-1}]
D_A [μm]


F=0.9, m=1.15, mp=0.0001
Cext_ho
Cext_ho_EB
Cext_sp
Cext_sp_EB
C_{ext} / V_M [μm^{-1}]
D_A [μm]

ADDING KHELIFA AND HILL (2006)

Khelifa and Hill model is used to determine fractal dimension as a function aggregate size: larger aggregates have lower fractal dimension. The model is a power law, defined as follows.

$d_3 = 3\left(\frac{D_A}{D_0}\right)^{\beta}$, where $\beta = \frac{\log(d_{3c}/3)}{\log(D_c/D_0)}$, and the parameters are defined as suggested by Khelifa and Hill based on extensive field data: primary particle size, $D_0 = 1\ \mu\mathrm{m}$, minimum fractal dimension, $d_{3c} = 2$, and the aggregate size for minimum fractal dimension, $D_c = 2000\ \mu\mathrm{m}$.

Fractal dimension is then converted to solids fraction, $F = \left(\frac{D_A}{D_0}\right)^{d_3-3}$.

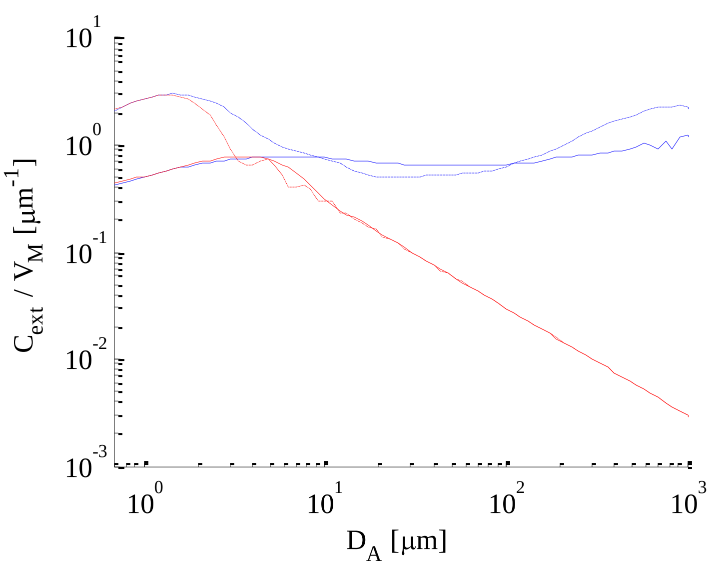
Implemented in KhelifaHill.m:

```
% Khelifa and Hill 2006
beta = log10(d3c./3)./log10(Dc./Dp);
d3 = 3.*(D_A./Dp).^beta;    % fractal dimension as function of aggregate size

F = (D_A./Dp).^(d3-3);  % solid fraction as function of aggregate size

V_M = F.*(pi/6).*D_A.^3;
```

Function returns the solids fraction, F, and the volume of solid mass, V_M.



Particulate beam attenuation normalized to solid volume for model aggregate (blue) and solid sphere (red) as a function of particle size. Solid and dashed lines represent particles with characteristic phytoplankton and inorganic composition, respectively.

MODEL RESULTS FOR POPULATIONS OF PARTICLES

See Boss, E., Slade, W.H., and P. Hill, 2009. Effect of particulate aggregation in aquatic environments on the beam attenuation and its utility as a proxy for particulate mass. Optics Express, Vol. 17, No. 11, pp. 9408-9420.