On the Aggregation Model of Marine Particles by Quadrature Method of Moments

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Marine particles contain organic particles which can grow, like algae and microbes, and inorganic particles, like colloids. The size distribution of the diameter of particles, from submicron scales to macroscopic scales, can be determined by factors like:

- The dynamic of marine ecological system
- Ocean currents
- Chemical reactions in ocean
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Why do we study it?

- It can affect the ecological state in a certain region of the ocean, like zooplankton grazing, vertical flux, light penetration, etc.
- It can affect the climate change and global warming, because it provides a way to get carbon from the surface ocean to the deep ocean, and so away from the atmosphere, and to be stored in the deep ocean for many thousands of years.
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Aggregation Processes in the Ocean Environment

Figure: Particles in the ocean environment

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Particle growth and aggregation processes can be described by an integro-differential equation which has been used previously to study marine particles (Hunt 1980, McCave 1984) as well as in industrial processes (Marchisio et al, 2003),

$$\frac{dn(D,t)}{dt} = \alpha \int_0^v \beta(\bar{v}, v - \bar{v}) n(v - \bar{v}, t) n(\bar{v}, t) \, dv - \alpha \int_0^\infty \beta(v, \bar{v}) n(v, t) n(\bar{v}, t) \, d\bar{v} + \frac{\partial}{\partial D} (G(D)n(D, t)), \tag{1}$$

where $v$ is the volume, (directly) proportional to $D^3$ for solid particles and $\beta(\bar{v}, v - \bar{v})$ is the coagulation kernel, measuring the frequency of particles’ coagulation.
The $k$-th moments of the size distribution at time $t$ is defined as

$$m_k(t) := \int_0^\infty D^k n(D, t) dD. \quad (2)$$

They have particular meanings, for instance, $m_0$ is the total number of particles, $m_2$ is (proportional to) the total surface area of particles, $m_3$ is (proportional to) the total solid volume, etc.
Let \( u^3 := D^3 - \delta^3 \), by multiplying \( D^k \) and integrating, one can get the equation of moments

\[
\frac{dm_k(D,t)}{dt} = \frac{\alpha}{2} \int_0^\infty n(\delta, t) \int_0^\infty \beta(\delta, u)n(u, t)(u^3 + \delta^3)^{\frac{k}{3}} \, du \, d\delta \\
- \alpha \int_0^\infty D^k n(D, t) \int_0^\infty \beta(D, \delta)n(\delta, t) \, d\delta \, dD \\
+ \int_0^\infty kG(D)n(D, t)D^{k-1} \, dD.
\]

(3)
Assuming that

\[ n(\delta, t) \approx \sum_{i=1}^{n} w_i(t) \delta(D - L_i(t)). \] (4)

and then using the approximation

\[ m_k(t) \approx \sum_{i=1}^{n} w_i(t) L_i^k(t). \] (5)

The main advantage of QMOM is that it allows us to close the system of equations and solve them for any kind of intial distributions.
Transformation of the Equation by QMOM

By the quadrature method of moments, the integro-differential equations can be transformed to ordinary differential equations

\[
\frac{dm_k(D,t)}{dt} = \frac{\alpha}{2} \int_0^\infty n(\delta, t) \int_0^\infty \beta(\delta, u)n(u, t)(u^3 + \delta^3)^k \frac{k}{3} dud\delta
\]

\[-\alpha \int_0^\infty D^k n(D, t) \int_0^\infty \beta(D, \delta)n(\delta, t)d\delta dD
\]

\[+ \int_0^\infty kG(D)n(D, t)D^{k-1}dD
\]

\[\approx \frac{\alpha}{2} \sum_{i=1}^3 w_i \sum_{i=1}^3 w_j \beta(L_i, L_j)(L_i^3 + L_j^3)^k
\]

\[-\frac{\alpha}{2} \sum_{i=1}^3 w_i L_i^k \sum_{i=1}^3 w_j \beta(L_i, L_j)
\]

\[+ k \sum_{i=1}^3 G(L_i)L_i^{k-1}w_i.
\]

(6)
The program of quadrature method of moments for the model contains:

1. Generate weights and abscissas from a moment (product-difference algorithm, Gordon, 1968);
2. Compose the program of generating weights ans abscissas into the ordinary differential equation system;
3. Set a time step and solve the ordinary differential equation system by Matlab’s ode solvers;
4. Put the solutions into the general output of moments for each time step.
Numerical Experiments for the Model

Assume the constant coagulation kernel, Brownian coagulation kernel, etc, in the equation. The Brownian kernel has the expression,

\[ \beta_{Br}(D, \tilde{D}) = c \left( \frac{1}{D} + \frac{1}{\tilde{D}} \right)(D + \tilde{D}), \]  

(7)

which is a coagulation kernel of the interaction between two particles with diameters \(D\) and \(\tilde{D}\) due to the Brownian motion in particle physics.

Figure:
Initial Size Distribution

Exponential spectrum

Figure: Initial Distribution: \( n(D) = 3D^2 \exp(-D^3) \)
Initial Size Distribution

Power law spectrum

Figure: Initial Distribution: \( n(D) = D^{-3} \)
Consider only the growth in the growth-aggregation equation.

Figure: Size-dependent growth for the power law initial spectrum
Considering only the aggregation, we have only the first two terms in the growth-aggregation equation.
Moments in the Growth-aggregation Process

For the exponential spectrum

Figure: Growth-aggregation with the initial exponential spectrum

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Moments in the Growth-aggregation Process

For the power law spectrum

Figure: Growth-aggregation with the initial power law spectrum
With the Brownian Kernel

Figure: With the Brownian kernel and exponential initial spectrum
Further Work

Consider the sinking process in the model, for which the equation will be

\[
\frac{dn(D,t)}{dt} = \frac{\alpha}{2} \int_0^v \beta(\bar{v}, v - \bar{v}) n(v - \bar{v}, t) n(\bar{v}, t) d\bar{v} \\
- \alpha n(v, t) \int_0^{\infty} \beta(v, \bar{v}) n(\bar{v}, t) d\bar{v} + \frac{\partial}{\partial D} (G(D) n(D, t)) \\
- n(D, t) \frac{w_s(D)}{h},
\]

(8)

where \(w_s(D)\) is the settling velocity and \(h\) is the depth.