Particle Dynamics in the Ocean:
Marine Particle Processes and their Representation

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Outline

- How do we describe particles?
- How do we represent particle dynamics?
**Martin Curve**

\[
F(z) = F_{100} \left( \frac{z}{100} \right)^b
\]

\[b = -0.973 \rightarrow -0.319\]

\[b = -0.858\]

Martin et al., 1987
Some Philosophy

- **Modeling as simulation**
  - *Reproduce the data*
  - *Fit simple functions*

- **Modeling as theory**
  - *Use first principles to make predictions*
  - *Allow for spatial & temporal variability*

- **Suite of models at different scales**
How to classify particles?

- Biogeochemical function
- Flux contribution
- Ecosystem function
- Particle Size
- Particle Settling Speed
- Particle Type
- ???
Particle Size Spectra

Jackson et al., 1997
and average size of aggregates drop off appreciably below the euphotic zone (Fig. 1), driving with them a drop in the total volume of aggregates per liter. This implies that degradation processes are strongly active in the upper few hundred meters and that processes in this zone bear considerable influence on the flux reaching deeper waters (Bishop et al., 1978, 1980).

Although cameras are a powerful means of investigating aggregates in the ocean, their instantaneous views of particle distributions may miss episodic pulses of material that contribute disproportionately to particle flux, such as events associated with phytoplankton blooms (Billett et al., 1983; Asper et al., 1992) or the breakdown of water-column stratification by convective mixing (Kemp et al., 2000). Such pulses of phytodetritus to the seafloor have been seen in all ocean basins in both coastal and open-ocean locations, and can, in the course of a few days to a few weeks, deliver the equivalent of the annual average carbon flux to the benthos (Beaulieu, 2002).

Fig. 1. Examples of aggregate number per liter, mean equivalent spherical diameter (ESD) for all particles, and volume of aggregates per liter (calculated from number and mean ESD) versus depth from video images. The upper panels depict one profile from the Southern Ocean at 48.9°S, 72.1°E (data from Gorsky and Picheral, 2004a). The middle panels show a profile from the eastern Atlantic at 20.5°N, 18.7°W (data from Gorsky, 2004) and the area in gray is below the detection limit of the camera. The bottom panels show a profile from the equatorial Pacific at 5.0°N, 179.8°W (data from Gorsky and Picheral, 2004b). A multitude of such data exist, for example, archived on Pangaea (http://www.pangaea.de/Info/).
Variations in spectral slope

Guidi et al., 2009
\[
\frac{dn(m, t)}{dt} = \frac{\alpha}{2} \int_0^m \beta(m_j, m - m_j)n(m - m_j, t)n(m_j, t) \, dm_j \\
- \alpha n(m, t) \int_0^\infty \beta(m, m_j)n(m_j, t) \, dm_j \\
- n(m, t) \frac{w_s(m)}{z} + I(m, t)
\]
Coagulation kernels

\[
\frac{dn(m, t)}{dt} = \alpha \int_0^m \beta(m_j, m - m_j) n(m - m_j, t) n(m_j, t) \, dm_j
\]

\[
- \alpha n(m, t) \int_0^\infty \beta(m, m_j) n(m_j, t) \, dm_j
\]

\[
- n(m, t) \frac{\nu_s(m)}{z} + I(m, t)
\]
Coagulation Mechanisms

**Brownian Motion**

\[ \beta(r_i, r_j) = \frac{2 kT}{3 \mu} \frac{(r_i + r_j)^2}{r_i r_j} \]

**Fluid Shear**

\[ \beta(r_i, r_j) = 1.3 \left( \frac{\epsilon}{\nu} \right)^{1/2} (r_i + r_j)^3 \]

\[ \beta(r_i, r_j) = \frac{p^2}{1 + 2p^2} \left( \frac{\epsilon}{\nu} \right)^{1/2} (r_i + r_j)^3 \]

**Differential Sedimentation**

\[ \beta(r_i, r_j) = \pi(r_i + r_j)^2 |w_j - w_i| \]

\[ \beta(r_i, r_j) = 0.5\pi r_j^2 |w_j - w_i| \]
Stickiness

\[
\frac{dn(m, t)}{dt} = \alpha \int_0^m \beta(m_j, m - m_j)n(m - m_j, t)n(m_j, t)\, dm_j \\
- \alpha n(m, t) \int_0^\infty \beta(m, m_j)n(m_j, t)\, dm_j \\
- n(m, t) \frac{\omega_s(m)}{z} + I(m, t)
\]

Stickiness: largely biological & chemical? Transparent exopolymer particles - nanogels?
of both tangles and weak, low-energy bonds (Verdugo 1990). These features make the assembly/dispersion dynamics of tangled networks depend primarily on polymer length—in fact, on the second power of the contour length of the assembled polymers (Edwards & Grant 1973). Assembly and dispersion are diffusion-limited processes. Longer flexible polymers have a higher probability of becoming entangled and forming networks. Conversely, dispersion of assembled networks requires that polymers randomly reptate (axially diffuse) their way out of the network. Diffusion times depend on the second power of the length of the random walk, which in this case is the length of the polymers. Thus, the stability of tangled networks and thereby the equilibrium size of tangle gels is critically limited by chain length (de Gennes & Léger 1982, Doi & Edwards 1998). Shorter polymers not only can walk out of tangles faster, but are likely to have a much lower number of low-energy cross-links. The resulting gels are smaller and short-lived. Axial reptational diffusion is also at the center of a critical feature of tangled networks—namely, it makes annealing between tangled gels possible. This is a paramount feature because it allows polymers from neighboring gels to interpenetrate their respective networks to form larger gels (Figure 1).

In short, low-energy interactions are an important additional factor that contributes to the stability of tangled gels. Physical gels reach an assembly/dispersion equilibrium that is reversible and depends not on specific chemical composition or complementary reactive residues but primarily on their concentration, and on physical features including charge density (ζ-potential), hydrophobic/hydrophilic domain ratios, flexibility, topology (linear, branched, star, etc.), quaternary conformation (globular, beta sheet, random coil, etc.), and particularly the size (contour length) of the polymer chains. Assembly also depends on the characteristics of the solvent—including dielectric

\[
\delta[NanoG]/\delta t = K_1[DOC] - K_2[DOC] - K_3[NanoG]_2 + K_4[SAG]
\]

\[
\delta[SAG]/\delta t = K_3[NanoG]_2 - K_4[SAG]
\]
Nano-gels

Polymers with stickiness varying along their length

Distribution of stickiness and polymer rigidity affects fractal dimension, gel size, aggregation times

\[
\frac{dn(m, t)}{dt} = \frac{\alpha}{2} \int_0^m \beta(m_j, m - m_j) n(m - m_j, t) n(m_j, t) \, dm_j \\
- \alpha n(m, t) \int_0^\infty \beta(m, m_j) n(m_j, t) \, dm_j \\
- n(m, t) \frac{w_s(m)}{z} + I(m, t)
\]
that much of the mass not represented by organic matter is composed of mineral ballast, the %OC results suggest that the OC:ballast ratio is slightly higher for more slowly settling material. During the second deployment, the %OC and %TN data displayed a fair amount of scatter (see analysis above), but the OC:TN ratios had a distinct step toward lower OC:TN values at SVs less than ~10 m d$^{-1}$, again suggesting enrichment in carbohydrate-like material at slow settling velocities.

NetTrap and elutriator—The free-drifting NetTrap was deployed several times at the DYFAMED site in May 2003 for time periods ranging between 19 and 72 h and, because of the short deployment durations, with no poisons or preservatives in the cod end. Although the NetTrap was designed to collect large amounts of material rather than to quantitatively measure flux, the particle “flux” collected by this trap at 200 m (170 mg m$^{-2}$ d$^{-1}$) was similar to fluxes measured by the moored 200-m arrays just before (153 mg m$^{-2}$ d$^{-1}$) and after (165 mg m$^{-2}$ d$^{-1}$) the NetTrap deployment. The NetTrap does not appear to collect suspended particles other than those in the trap at the time that it is closed. No particles were visible on the net walls after recovery, and the net was recovered in the closed position, so no particles would have been collected during ascent.

The large amount of material collected by the NetTrap allowed elutriation of the particles by SV into discrete classes. In these initial trials, the elutriator was operated with a water flow that separated particles into five fractions of >230, 230-115, 115-58, 58-29, and <29 m d$^{-1}$. Particles with settling rates of <29 m d$^{-1}$ were removed from the flow stream using a flow-through centrifuge. The elutriated mass was distributed into the 5 fractions as 57.2%, 13.4%, 1.54%, 4.74%, and 23.1% of the total (Fig. 7). Hence, 80% of the elutriated mass had SV >115 m d$^{-1}$, consistent with the sinking velocity/mass flux profiles of the SV traps (62% of total mass flux sank at >98 m d$^{-1}$; Figs. 2 and 6A, tubes 2-5).

The %OC in the elutriated fractions followed the inverse pattern as mass (Table 2; Fig. 7). The OC composition (20%) in the NetTrap samples was more similar to the higher values found in the later trap period between mid-May and July. Results showing differences in radionuclide and lipid composition and lability with respect to decomposition between elutriator stages are available on the MedFlux web site (see above) and will be published elsewhere.

We compared mass flux densities of elutriated particles with those separated by SV-IRS traps. Because the settling-velocity intervals of the elutriator and SV-IRS were not the same, a comparison requires that mass fluxes be normalized for the different settling velocities. We accomplished this by dividing mass fluxes in each settling-velocity interval by $\log_{10}(SV_{\text{max}}) - \log_{10}(SV_{\text{min}})$ for that interval (Fig. 8). In this way, the area of each column represents mass flux, and the height of the column is the flux density, $d_{\text{flux}}/d\log_{10}(SV)$. As shown in Fig. 8, the May elutriator results fell between the March-May and May-June SV-IRS results.

**Peterson et al., Limnol. Oceanogr. Methods, 2005**

**McDonnell & Buesseler, Limnol. Oceanogr., 2011**
\[
\frac{dn(m, t)}{dt} = \frac{\alpha}{2} \int_0^m \beta(m_j, m - m_j)n(m - m_j, t)n(m_j, t) \, dm_j \\
- \alpha n(m, t) \int_0^\infty \beta(m, m_j)n(m_j, t) \, dm_j \\
- n(m, t) \frac{w_s(m)}{z} + I(m, t)
\]
Sectional Approach

n₁  n₂  n₃  n₄  n₅
Mass Balance

Total System Mass Balance: Steady State Value = 1

Cagulation losses/settling losses: Steady State Value = 2.6765e−08
Integral Models

Mass concentration
\[
\frac{d\phi}{dt} = \mu\phi - \frac{F_{\phi}}{Z}
\]

Number concentration
\[
\frac{d\psi}{dt} = \mu\psi - \frac{F_{\psi}}{Z} - \xi
\]

\[
F_{\psi} = \int_{d_0}^{\infty} w(d)n(d) \, dd
\]
\[
F_{\phi} = \int_{d_0}^{\infty} C(d)w(d)n(d) \, dd
\]
\[
\xi = \frac{\alpha}{2} \int_{d_0}^{\infty} \int_{d_0}^{\infty} \left( \beta_{\text{shear}}(d_1, d_2) + \beta_{\text{ds}}(d_1, d_2) \right) n(d_1)n(d_2) \, dd_1 \, dd_2
\]
\[
n(d) = Ad^{-e}
\]

Based on Kriest & Evans, *Earth & Planetary Sciences*, 2000
Size spectrum comparison

![Graph showing size spectrum comparison]

- Sectional Initial
- Integrated Initial
- Sectional Final
- Integrated Final
Diameter [cm]

N [cm$^{-3}$ per size class]

Sectional Initial
Integrated Initial
Sectional Final
Integrated Final
Flux Comparison

Diameter [cm]

Mass Flux [nmol cm\(^{-2}\) d\(^{-1}\)]

- Sectional Initial
- Integrated Initial
- Sectional Final
- Integrated Final

Diameter [cm]
Biological Processes

Stemmann et al., *Deep-Sea Research I*, 2004
Chemical Processes

Extension of Honeyman & Santschi (1989)

Burd et al., Deep-Sea Research I, 2000
Multiple Particle Types

Three particle types (algal cells, fecal pellets, aggregates)

Each follows a separate log-normal distribution.

Each particle type has settling velocity law, carbon content etc.

Burd et al., Deep-Sea Research I, 2007
Multiple Particle Types

Coagulation coupled to an ecosystem model

Jackson, Deep-Sea Research I, 2001
Conclusions

🌿 Need a combination of modeling approaches
- Detailed mechanistic models & data comparisons on the same scales & same information
- Computationally efficient models that capture the dynamics and can run in large scale models

🌿 Need to assess the assumptions built into the models
- How do assumptions (scientific & numerical) affect interpretation of results?

🌿 Models & data need to inform each other