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Rapid formation of large aggregates during the spring bloom of Kerguelen Island: observations and model comparisons

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Supplement S1: Model description

The biological model for phytoplankton growth is a modified form of that in Evans and Parslow (1985) and Fasham *et al* (1990). In this case, there is only one nutrient, nitrate, and phytoplankton are lost to coagulation as in Jackson (1995) and Jackson et al. (2005). There are no grazing losses. Values for constants are given in Table 1.

Nitrate concentration

Change in nitrate concentration N:

$$\frac{\partial N}{\partial t} = K_z \frac{\partial^2 N}{\partial z^2} - G\phi \qquad \text{(A1.)}$$

where K_z=vertical mixing coefficient, G is the phytoplankton specific growth rate, and φ is the phytoplankton concentration.

Phytoplankton growth

Phytoplankton growth rate at any given irradiance and nutrient concentration is given by

$$G = G_{max}\ \min(r_p, r_n) \qquad \text{(A2.)}$$

where $G_{max}$is the maximum specific growth rate, r_p and r_n are the relative growth rates possible growth for photosynthesis and nutrient limitation at I and N. They are calculated by

$$r_p = \frac{\alpha_I I}{\sqrt{\alpha_I{}^2 I^2 + G_{max}^2}} - \frac{r}{G_{max}} \qquad \text{(A3.)}$$

where r is the phytoplankton loss rate and α is the slope of the PI curve.

$$r_n = \frac{N}{K_D + N} \qquad \text{(A4.)}$$

where K_D is the half saturation constant for nitrate uptake.

Irradiance I given by

$$I = I_0 e^{\int_0^z k dz} \qquad \text{(A5.)}$$

where I_0 is the surface irradiance, $k = k_w + \varphi\ k_r$, k_w is the attenuation coefficient for water and 0.04 m^{-1} and k_r is the light absorption coefficient for plants. The value of k_r was chosen so that k equaled the observed attenuation at A3 (k=0.048 m^{-1} for P = 0.6 µg chl/L). Surface irradiance was calculated using the relationships of Evans and Parslow (1985) for a latitude of 50°S and a starting time 120 d after winter solstice.

A single phytoplankton cell was assume to have a diameter of 20 um and a density of 1.0637 g cm^{-3} (compared to a fluid density of 1.0275 g cm^{-3}), for a resulting settling speed of 1.05 m d^{-1}.

Describing particle size distributions

Standard coagulation theory describes particle size distributions using a number spectrum *n(s)*, where *s* is particle size, such as mass *m* or equivalent spherical diameter *d*. Number spectra in terms of *m* and *d* can be related

$$n(d) = n(m)\frac{dm}{dd} \tag{A6.}$$

The total number of particles in a small size interval $d_l < d \leq d + \Delta d$ is approximately $n\ \Delta d$. For a sufficiently small Δd, all particles have the same individual volume $V(d) = \frac{\pi}{6}d^3$. The total particle volume in the interval is then $V(d)\ n\ \Delta d$. The total particle volume for any large particle range $d_l < d \leq d_u$ is

$$V_T = \int_{d_l}^{d_u} V(d)n(d)\mathrm{d}d \tag{A7.}$$

which is proportional to the area under the curve when nV is plotted as a function of *d*. Plotting nV versus the logarithm of *d* destroys the relationship between the area under the curve and the total particle volume; plotting nVd as a function of log *d* restores it. We will discuss particle size distributions in terms of the nVd form of the distribution, but note that it contains the same content as *n*.

How coagulation changes size distributions

Coagulation destroys small particles and creates new ones in a way that is mathematically expressed as

$$\frac{\partial n(m,t)}{\partial t} = +\alpha \int_0^m n(m_1)n(m-m_1)\beta(m_1, m-m_1)dm - \alpha n(m)\int_0^\infty n(m_1)\beta(m,m_1)dm_1 \tag{A8.}$$

where $\beta(m_1, m_2)$ is the coagulation kernel and describes the collision rate between particles of masses m_1 and m_2 and α is the stickiness, the probability of a collision destroying the two colliding particles and forming a larger particle.

One of the techniques for solving this equation numerically is to break the size distribution *n* into segments, called sections, each with a fixed shape but a variable magnitude, such that

$$n(m,t) = \frac{Q_i(t)}{\widehat{m}_{l-1}m} \tag{A9.}$$

within a range of $\widehat{m_l} > m \geq \widehat{m}_{l-1}$, where $Q_i(t)$ is the total particulate mass within the bounds (e.g., Jackson 1995) and the range represents the section boundaries. This approximation breaks *n(m,t)* into separate time and mass varying parts. Gelbard et al. showed that doing so allows Eq. A8 to be transformed from an integer-differential equation to a series of ordinary differential equations:

$$\frac{dQ_l}{dt} = \frac{\alpha}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1} {}^1\bar{\beta}_{i,j,l}\ Q_iQ_j - \alpha Q_l \sum_{i=1}^{l-1} {}^2\bar{\beta}_{i,l}Q_i - \frac{\alpha}{2}\ {}^3\bar{\beta}_{l,l}Q_l^2 - \alpha\ Q_l \sum_{i=l+1}^{l_{max}} {}^4\bar{\beta}_{i,l}Q_i \tag{A10.}$$

where ${}^1\beta_{i,j,l}$, ${}^2\beta_{i,l}$, ${}^3\beta_{l,l}$, and ${}^4\beta_{i,l}$ are sectional coefficients and l_{max} is the total number of sections. The equations simplify if the mass of the upper boundary of a section is twice that of its lower boundary.

Jackson (1995) added a disaggregation term to Eq. A10 which moved mass from section *i* to the next lower section *i-1* at a rate $\lambda_i Q_i$, where λ_i is a size dependent disaggregation coefficient. We used the values for λ_i from Jackson(1995).

The algae were assumed to be occupy the first section: $\varphi = Q_1$. The equation describing their concentration is

$$\frac{\partial Q_1}{\partial t} = Q_1 G + v_1 \frac{\partial Q_1}{\partial z} - K_z \frac{\partial^2 Q_1}{\partial z^2} - \frac{\alpha}{2}\, {}^3\bar{\beta}_{1,1} Q_1^2 - \alpha\, Q_1 \sum_{i=2}^{l_{max}} {}^4\bar{\beta}_{i,1} Q_i \; + \lambda_2 Q_2 \qquad \text{(A11.)}$$

For particles in larger sections, the equation describing their concentration becomes

$$\frac{\partial Q_l}{\partial t} = v_l \frac{\partial Q_l}{\partial z} - K_z \frac{\partial^2 Q_l}{\partial z^2} + \lambda_{l+1} Q_{l+1} - \lambda_l Q_l + \frac{\alpha}{2} \sum_{i=1}^{l-1} \sum_{j=1}^{l-1} {}^1\bar{\beta}_{i,j,l}\; Q_i Q_j \qquad \text{(A12.)}$$

$$- \alpha Q_l \sum_{i=1}^{l-1} {}^2\bar{\beta}_{i,l} Q_i - \frac{\alpha}{2}\, {}^3\bar{\beta}_{l,l} Q_l^2 - \alpha\, Q_l \sum_{i=l+1}^{l_{max}} {}^4\bar{\beta}_{i,l} Q_i$$

where v_l is the settling rate for particles in the *l*th section.

Measures of aggregate size.

Because aggregate porosity increases with size, particle density decreases as particle size increases. The relationship between the diameter assigned to a particle from analysis of an image d_a is frequently described using a fractal dimension D_f: $m \propto d_a^{D_f}$. Increasing D_f decreases the porosity of large particles and results in smaller values of d_a for a given *m*. An apparent volume for a sphere with diameter d_a is then $V_a = \frac{\pi}{6} d_a^3$. A conserved volume V_c can be calculated from a particle's mass and the density of the single cell. Its diameter d_c can be calculated assuming it is a sphere.

Numerical solution of equations

The equations were solved numerically for a 150 m mixed layer using a centered-difference scheme, no-flux boundary conditions at the surface, fixed nitrate concentration= 30 µM and no diffusive particle flux at the bottom boundary (150 m). Equations were solved at a vertical spacing of 2 m. Particle concentrations were calculated in terms of the conserved volume.

Parameter values are given in Table 2.