Model calibration for aggregation-sedimentation dynamics

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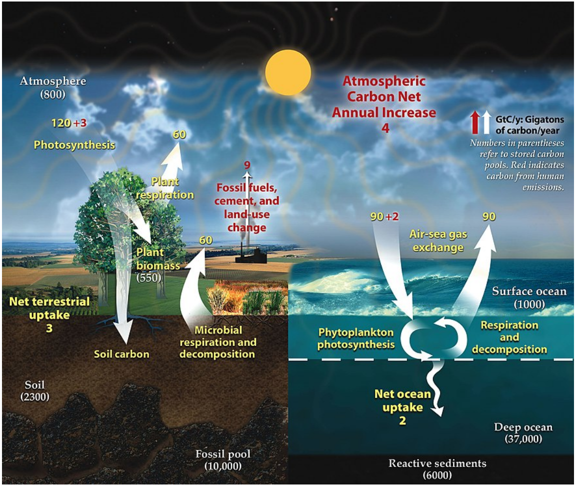
Universidad de Granada

CEDYA/CMA,
14-18 June 2021, Gijón and elsewhere

Global warming and the carbon cycle



(US government)

Transparent Exopolymeric Particles

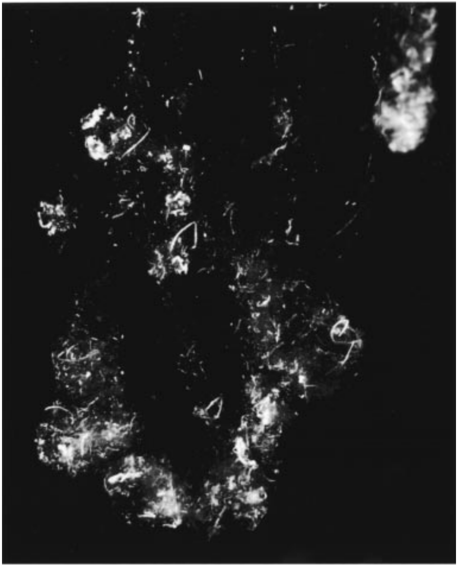
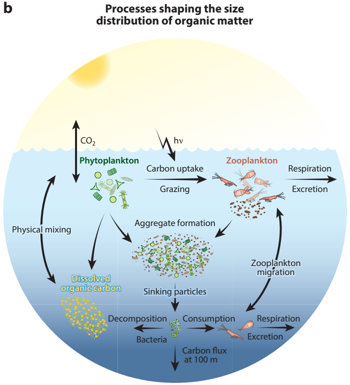


FIGURE 1. Picture of marine snow aggregate taken in situ, courtesy of A. L. Alldredge. The aggregate is about 1 cm across. It is composed primarily of marine diatoms, although fecal pellets can also be seen on it. The aggregate is held together with transparent material, presumable TEP. Several smaller aggregates can be identified as part of it, as can extensive void regions. Reprinted from cover photograph of *Deep-Sea Res. II*, Vol. 42, No. 1, 1995, with permission from Elsevier Science.

Predictive modeling in Aquatic Sciences



- Too many interactions going on at the same time
- Wide range of spatial and temporal scales involved
- Mastering different disciplines is needed
- Experimental data are not that easy to obtain

Size-class models

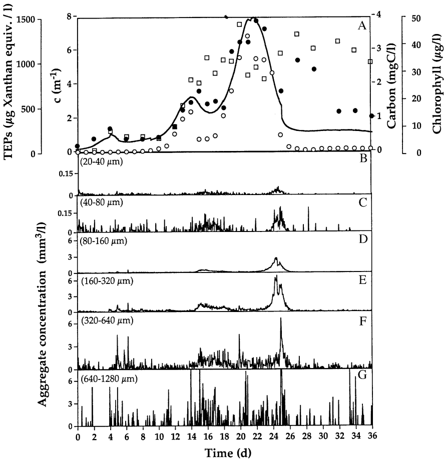


Fig. 1. (A) Time series of chlorophyll (open circles), POC (filled circles), TEP (squares) and beam attenuation (c; continuous line). (B)–(G) Represent volume concentration of aggregates during the experiment.

(Ruiz, Prieto, Ortegón, Deep-Sea Res. 49 (2002))

$$\frac{\mathrm{d}C_1}{\mathrm{d}t} = C_1 \sum_{j=1}^{7} \beta_{11j} C_j + \sum_{i=1}^{7} \eta_{1i} C_i$$

$$+ \text{primary production},$$

$$\frac{\mathrm{d}C_k}{\mathrm{d}t} = \sum_{i=1}^{7} \sum_{j=1}^{7} \beta_{kij} C_i C_j + \sum_{i=k}^{7} \eta_{ki} C_i,$$

$$J(\mathbf{s}) = \frac{1}{2} \int_{\theta_0}^{\theta_0+\Theta} \left[\sum_{i=1}^{7} (\mathbf{y}(\theta) - \hat{\mathbf{y}}(\theta))^2 \right] \mathbf{q}(\theta)\, \mathrm{d}\theta + Z(\mathbf{s}), \quad \text{(C.2)}$$

where Z is a penalization function. The optimization problem consists of finding the elements of $\mathbf{s}$ that minimize J and is treated via the conjugate gradient algorithm (Glowinski, 1984). The func-

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Size-spectrum models: the coagulation equation

$$\frac{\partial n(t,x)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)n(t,x-y)n(t,y)\,dy - \int_0^\infty K(x,y)n(t,x)n(t,y)\,dy\,.$$

- x is a measure of *size*
- Binary interactions $(x) + (y) \to (x+y)$
- $K(x,y)$ binary coagulation kernel

Plus additional terms, e.g.:

- sedimentation: $-n(t,x)w(x)/Z$
- synthesis: $+I(t,x)$
- binary or multiple fragmentation

(Burd, Jackson, Moran, Lochmann, Mari, Stemann, Ianson)

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The coagulation equation

- Aggregate number: $m_0(t) = \int_0^\infty n(t,x)\,dx$
- Volume (mass): $m_1 = \int_0^\infty x\, n(t,x)\,dx$

Gelling kernels: there exists $T_g \geq 0$ such that $m_1(t) = m_1(0)$ for each $t \in [0, T_g)$ and $m_1(t) < m_1(0)$ for $t > T_g$.

Kernels such that $K(x,y) \leq C(1 + x + y)$ are non-gelling.
For those we have:

- $m_1(t)$ is preserved.
- $m_0(t)$ decays to zero as $t \to \infty$.

The coagulation equation: some kernels

Brownian kernel: $\beta_{Br}(x,y) \simeq c(x^{1/3}+y^{1/3})(x^{-1/3}+y^{-1/3})$

Shear kernel: $\beta_{sh}(x,y) \simeq c(x^{1/3}+y^{1/3})^3$

Differential sedimentation kernel:
$\beta_{sed}(x,y) \simeq c(x^{1/3}+y^{1/3})^2|x^{1/3}-y^{1/3}|$

- Rectilinear and curvilinear formulations
- Fractal dimensions
- Bio-chemical interactions, etc

Modeling from first principles vs (nonparametric?) calibration

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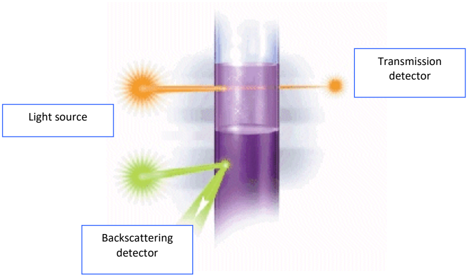
Modeling from first principles vs (nonparametric?) calibration

Pantano de Cubillas

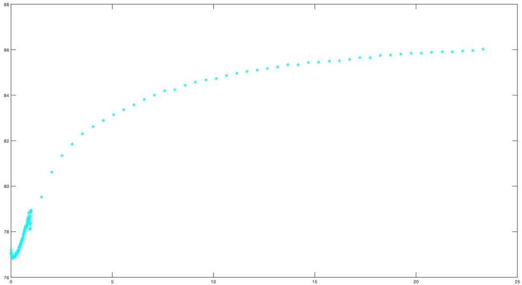
(Wikipedia: Enrique Íñiguez)

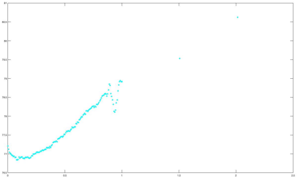
Measurement principle

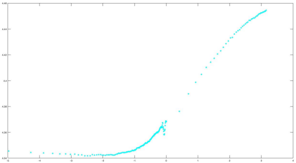


(IESMAT)

Sample measurements







Temporal dynamics for the average size

Lambert–Beer's law

$$T = T_0 \exp\left(\frac{-3r_i\phi Q_s}{d}\right)$$

$d = d(t)$ average particle diameter

For a constant coagulation kernel $K(x, y) = K$:

$$d(t) = \kappa_1(1 + \kappa_2 t)^{1/3}$$

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$$\mathrm{vol}(t) = \frac{m_1}{m_0(t)} \quad \text{and} \quad \frac{d\,m_0}{dt} = -\frac{K}{2}m_0^2.$$

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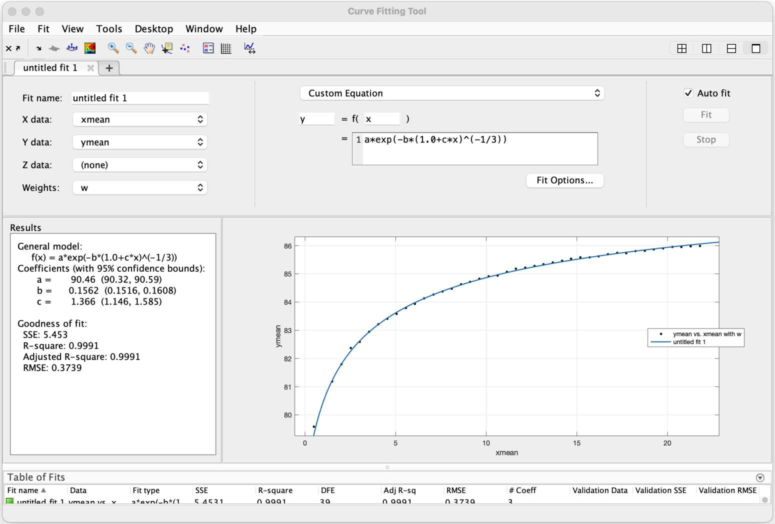
$$\mathrm{vol}(t) = \frac{m_1}{m_0(0)} + \frac{m_1 K}{2} t \quad \text{and} \quad d(t) = \left(\frac{6}{\pi}\mathrm{vol}(t)\right)^{1/3} .$$

Sample fits


Curve Fitting Tool
File Fit View Tools Desktop Window Help
untitled fit 1
Fit name: untitled fit 1
X data: xmean
Y data: ymean
Z data: (none)
Weights: w
Custom Equation
y = f(x)
= 1 a*exp(-b*(1.0+c*x)^(-1/3))
Fit Options...
Auto fit
Fit
Stop
Results
General model:
f(x) = a*exp(-b*(1.0+c*x)^(-1/3))
Coefficients (with 95% confidence bounds):
a = 90.46 (90.32, 90.59)
b = 0.1562 (0.1516, 0.1608)
c = 1.366 (1.146, 1.585)
Goodness of fit:
SSE: 5.453
R-square: 0.9991
Adjusted R-square: 0.9991
RMSE: 0.3739
ymean
xmean
ymean vs. xmean with w
untitled fit 1
Table of Fits
Fit name Data Fit type SSE R-square DFE Adj R-sq RMSE # Coeff Validation Data Validation SSE Validation RMSE

Recovering $K(x, y)$: homogeneous kernels

There exists $\lambda > 0$ such that $K(\gamma x, \gamma y) = \gamma^\lambda K(x, y), \ \forall \gamma > 0$.

Therefore, $K(x, y) = y^\lambda \kappa(x/y) = x^\lambda \kappa(y/x)$.

Dynamical scaling hypothesis

For homogeneous kernels the long time behavior of the coagulation equation is *self-similar*, that is,

$$n(t, x) \sim t^{2\nu} g(t^\nu x) \quad (\text{here } \nu = -\frac{1}{1-\lambda} < 0)$$

$$2g(z) + zg'(z) + \frac{\lambda - 1}{2} \int_0^z K(z-y, y) g(z-y) g(y)\, dy$$

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Inverse problem for the coagulation kernel

$$f(z) := \frac{1}{m_1} \int_0^z w\, g(w)\, dw \, ,$$

$$\frac{\nu}{m_1} z\, f'(z) = \int_0^1 \kappa(\xi)\Omega(\xi, z)\, d\xi$$

$$\Omega(\xi, z) := -\int_{\frac{z}{1+\xi}}^{z/\xi} y^\lambda f'(y) f'(y\,\xi)\, dy - \frac{1}{\xi} \int_{\frac{z}{1+\xi}}^{z} y^\lambda f'(y) f'(y\,\xi)\, dy \, .$$

(Muralidhar, Ramkrishna, Wright, Tobin)

Inverse problem for the coagulation kernel

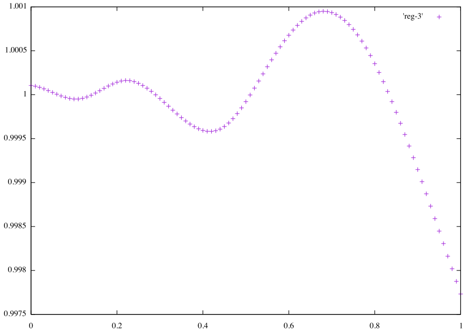
1. Collocation points: $z_i \in [2^{-8}, 2^2]$, logarithmically spaced
2. B-splines in $[0,1]$: $\kappa(\xi) = \sum_{i=1}^{p} c_i \beta_i(\xi)$
3. Overdetermined system: $X\, c^T = d$
   with $x_{ij} = \int_0^1 \beta_j(\xi)\Omega(\xi, z_i)\, d\xi$ and $d_i = \frac{\nu}{M_1} z_i f'(z_i)$
4. Regularization: $\min_c \|Xc^T - d\|_2^2 + \lambda\, cWc^T$
5. Reduction to standard form: $W = L\, L^T$ and set $u^T = L^T\, c^T$
6. Solve via SVD: $XL^{-1} = UDV^T$

(Muralidhar, Ramkrishna, Wright, Tobin)

Test-bed case

Constant kernel ($\lambda = 1$)

$\nu = -1$ and $g(z) = \frac{4}{m_1} e^{-\frac{2z}{m_1}}$. Thus, $f'(z) = \frac{4z}{m_1^2} e^{-\frac{2z}{m_1}}$.



$$w_{ij} = \int_0^1 \beta_i(\xi)\,\beta_j(\xi)\ d\xi + \int_0^1 \beta_i'(\xi)\,\beta_j'(\xi)\ d\xi + \int_0^1 \beta_i''(\xi)\,\beta_j''(\xi)\ d\xi$$

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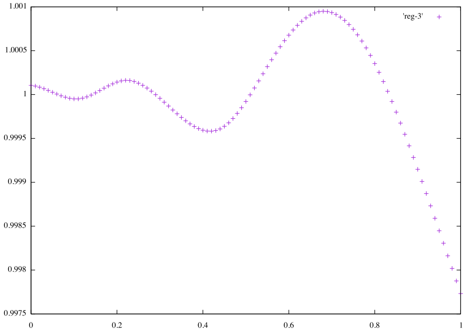

$$w_{ij} = \int_0^1 \beta_i(\xi)\,\beta_j(\xi)\; d\xi + \int_0^1 \beta_i'(\xi)\,\beta_j'(\xi)\; d\xi + \int_0^1 \beta_i''(\xi)\,\beta_j''(\xi)\; d\xi$$

Recap

- Aggregation in aquatic contexts is an important mechanisms influencing the global carbon cycle.
- A wide collection of processes are supposed to mediate aggregation interactions. Reverse-engineering approaches can be worth trying.
- Aggregation in lakes and reservoirs: a constant coagulation kernel may be accurate enough.

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