ESTIMATION OF THE RATES OF PARTICLE (DIS)AGGREGATION IN THE MESOPELAGIC ZONE OF THE EASTERN NORTH PACIFIC

A progress Report

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The overarching goal of this research is to extract information about the dynamics of particles in the ocean mesopelagic zone (100 – 1000 m) from measurements of the concentration of particulate organic carbon (POC), lithogenic elements (Al and Ti), and thorium-234 (a particle-reactive radioisotope).

Measurements of POC, Al, Ti, and thorium-234 in different size fractions have been obtained in the upper 500 m of the water column in the Gulf of Alaska during summer 2018 as part of a cruise of the NASA EXPORTS program.

Here we present the status of our effort to use the size-fractionated POC measurements from the EXPORTS cruise in order to estimate the rates of particle sinking, remineralization, aggregation, and disaggregation of a 1D (vertical) model of particle cycling in the upper mesopelagic zone.

To this end, we apply an inverse method that allows for the consideration of the errors both in the POC data and in the model and that provides approximate estimates of the errors in the rate parameters.
The rates at which organic particles sink, remineralize, aggregate, and disaggregate influence the export of organic carbon from surface waters to deep waters (“biological carbon pump”).

Figure from Lam & Marchal (2015)
• Sampling near Ocean Station Papa, a high-nutrient low-chlorophyll (HNLC) region of the ocean.

• Size-fractionated samples collected via Large Volume In Situ Filtration (pumps)

• Three size fractions collected, grouped into 2 size fractions for this study:
  - small size fraction, SSF (1-51 µm)
  - large size fraction, LSF (>51 µm)

Map showing the location of Ocean Station Papa (OSP), the ship track (line P), and the major currents in the region. Modified from Freeland (2007).
Temperature and salinity profiles measured at OSP during the EXPORTS North Pacific cruise

- Depth of mixed layer ~30 m
- Depth of euphotic zone (0.1% PAR) ~115 m
- Sharp halocline

Temperature and salinity profiles measured at OSP during the EXPORTS North Pacific cruise

unpub. data from EXPORTS group
NUMERICAL MODEL OF POC CYCLING: key features

- Model domain: from 30 m (base of mixed layer) to 500 m (deepest sample)
- Model grid: regular grid with $\Delta z = 5$ m
- Model assumptions:
  - steady state
  - one-dimensionality
  - all transport processes omitted except particle sinking
  - particle aggregation described with 2nd-order kinetics
  - vertically uniform rate parameters except $\beta_{-1,s}$*

* rate constant for the remineralization of SSF particles
NUMERICAL MODEL OF POC CYCLING: schematic

state variables

\( P_S \): [POC] in small size fraction (SSF)
\( P_L \): [POC] in large size fraction (LSF)

Parameters (r.c. = rate constant)

\( \dot{P}_S \): production rate of small particles
\( w_S \): sinking rate of small particles
\( w_L \): sinking rate of large particles
\( \beta_{-1,s} \): r.c. for small particle remineralization
\( \beta_{-1,l} \): r.c. for large particle remineralization
\( \beta_{-2} \): r.c. for small particle aggregation
\( \beta_{-1,l} \): r.c. for large particle disaggregation
NUMERICAL MODEL OF POC CYCLING: balance equations

Small particles:

\[ \frac{dP_S}{dz} = \dot{P}_s + \beta_{-2}P_l - \beta'_2P_s^2 - \beta_{-1,s}P_s \]

- Production
- Aggregation
- Settling
- Disaggregation
- Remineralization

Large particles:

\[ \frac{dP_l}{dz} = \beta'_2P_s^2 - \beta_{-2}P_l - \beta_{-1,l}P_l \]

- Aggregation
- Remineralization
- Settling
- Disaggregation
NUMERICAL MODEL OF POC CYCLING: treatment of particle production

\[ \dot{P}_s(z) = \bar{P}_s \exp \left( -\frac{z - z_{ML}}{L_p} \right) \]

where

- \( \bar{P}_s \) production rate of small particles in the mixed layer
- \( L_p \) vertical scale of variation for small particle production
- \( z_{ML} \) depth of the mixed layer (\( z_{ML} = 30 \) m)
All rate constants of the model except the rate constant for the remineralization of small particles, $\beta_{-1.5}$, are assumed to be uniform in the upper 500 m.

Motivated by independent evidence, the rate constant $\beta_{-1.5}$ is allowed to vary between four different layers in the upper 500 m:

- Layer A: 0 to 30 m
- Layer B: 30 to 115 m
- Layer C: 115 to 300 m
- Layer D: 300 to 500 m
DATA TREATMENT

- Measurements of POC in SSF & LSF from 12 different stations are averaged to produce a station-mean profile of POC in SSF & a station-mean profile of POC in LSF for the whole cruise.

- The station-mean profiles of POC in SSF & LSF are each vertically interpolated onto the model grid using a minimum-variance procedure.

- In this procedure, the covariances between the POC concentrations at different depths, say $z_i$ and $z_j$, are computed from

$$
\text{cov}[P_s(z_i), P_s(z_j)] = \sigma_s^2 \exp\left(-\frac{|z_i - z_j|}{L}\right) \quad \text{cov}[P_l(z_i), P_l(z_j)] = \sigma_l^2 \exp\left(-\frac{|z_i - z_j|}{L}\right)
$$

where

- $\sigma_s^2 = \text{variance of POC data in SSF}$
- $\sigma_l^2 = \text{variance of POC data in LSF}$
- $L = \text{vertical covariance scale for POC}$
The unknowns of the inverse problem include the parameters of the POC cycling model.

Since POC data contain errors, \( P_s \) and \( P_l \) in the POC cycling model are not perfectly known and should also be considered as unknowns of the inverse problem.

Accordingly, the vector of unknowns of the inverse problem is

\[
x = (w_s, w_l, \beta_{-1,s}, \beta_{1,s}, \beta_{-1,l}, \beta_{-2}, \beta_{-2}, \bar{P}_s, L_p, P_{s,1}, \ldots, P_{l,1}, \ldots)^T
\]

The vector \( x \) includes 95 values of \( P_s \) and 95 values of \( P_l \), since the numerical model includes 95 values of \( P_s \) and 95 values of \( P_l \) (one of such values per grid point).
Our goal is to find an estimate of $\mathbf{x}$ that is consistent with (i) prior estimates of model parameters from the literature, (ii) prior estimates of $P_s$ and $P_l$ from the POC data (interpolated values), and (iii) the POC cycling model, given estimates of the errors in (i), (ii), and (iii).

Mathematically, an estimate of $\mathbf{x}$ is sought that minimizes the following cost function,

$$ J = (\mathbf{x} - \mathbf{x}_0)^T \mathbf{C}_o^{-1} (\mathbf{x} - \mathbf{x}_0) + \mathbf{f}(\mathbf{x})^T \mathbf{C}_f^{-1} \mathbf{f}(\mathbf{x}) $$

where

- $\mathbf{x}_0$ vector containing the prior estimates of model parameters, $P_s$, and $P_l$
- $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ vector containing the (discretized) equations of POC cycling model
- $\mathbf{C}_o$ matrix containing the error (co)variances of the prior estimates in $\mathbf{x}_0$
- $\mathbf{C}_f$ matrix containing the error (co)variances of the model equations

We assume $\mathbf{C}_f = \gamma \mathbf{f}(\mathbf{x}_0)^T \mathbf{f}(\mathbf{x}_0) \mathbf{I}$

where $\gamma$ is the trade-off parameter and $\mathbf{I}$ is the identity matrix.
• The inverse problem is nonlinear since some of the unknowns appear as products in the equations of the POC cycling model (consider, for example, $\beta_{-2}P_1$).

• The solution of the inverse problem is obtained from an iterative procedure called the method of total inversion*. In this procedure, the model equations are linearized about the most recent estimate of $\hat{x}_k$, where $k$ is the iteration step.

• The estimated vector of unknowns at the $(k + 1)$th iteration is

$$\hat{x}_{k+1} = x_o + C_o F_k^T (F_k C_o F_k^T + C_f)^{-1} (F_k [\hat{x}_k - x_o] - f_k)$$

where $F_k = \text{matrix of partial derivatives of } f(x)\text{ with respect to } x\text{ evaluated at } x = x_k$

$f_k = \text{vector of functions } f(x)\text{ evaluated at } x = x_k$

• The covariance matrix for $\hat{x}_{k+1}$ is approximated from

$$C_{k+1} = \left[I - C_o F_k^T (F_k C_o F_k^T + C_f)^{-1} F_k\right] C_o \left[I - C_o F_k^T (F_k C_o F_k^T + C_f)^{-1} F_k\right]^T$$

* Tarantola & Valette (1982)
The solution with $\gamma = 1$ assumes a relatively low confidence in the POC cycling model.
The solution with $\gamma = 0.01$ assumes a relatively high confidence in the POC cycling model.
PARTICLE CYCLING RATES ESTIMATED BY DATA INVERSION ($\gamma = 0.01$)

**Preliminary Results:**

*Left panel:* small particle remineralization rates (SRemin) > small particle aggregation rates (Agg)

*Right panel:* large particle disaggregation rates (Disagg) > large particle remineralization rates (LRemin)
CONCLUSIONS

• Particle processes, such as aggregation and disaggregation, influence the export of organic C from surface to deep waters (biological C pump) and yet are poorly understood.

• Measurements of POC, Al, Ti, and $^{234}$Th concentrations in different size fractions have been obtained in the upper mesopelagic zone near Ocean Station Papa in the Gulf of Alaska during summer 2018 as part of NASA EXPORTS.

• POC concentrations measured on small and large size fractions collected in situ by filtration showed generally a decrease with depth in the upper 100 m at EXPORTS stations.

• The observed station-mean profiles of POC in both size fractions are used to estimate the parameters of a steady-state, 1D model of POC cycling in the mesopelagic zone of the ocean. To this aim, an inverse method that considers data & model errors and that provides approximate error estimates for model parameters is applied.

• Preliminary results suggest that, assuming relatively small model errors, particle processes proceed at noticeably different rates and variably influence the POC budgets in the upper 500 m.

• Future work will consider (i) POC data with high vertical resolution derived from beam transmissometry (light attenuation) and (ii) trace element data (Al, Ti, $^{234}$Th), to provide further constraints on particle processes at EXPORTS stations.
MODEL PARAMETERS ESTIMATED BY DATA INVERSION

\[ x_0 \] prior estimate
\[ \hat{x}(I) \] estimate obtained by neglecting data & model errors
\[ \hat{x}(II) \] estimate obtained by considering data errors only
\[ \hat{x}(III) \] estimate obtained by considering data errors & model errors (\( \gamma = 1 \))
\[ \hat{x}(IV) \] estimate obtained by considering data errors & model errors (\( \gamma = 0.01 \))