UC SANTA CRUZ

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

A progress Report

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GOAL OF THIS RESEARCH

- 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.

PARTICLE DYNAMICS & BIOLOGICAL CARBON PUMP

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”)

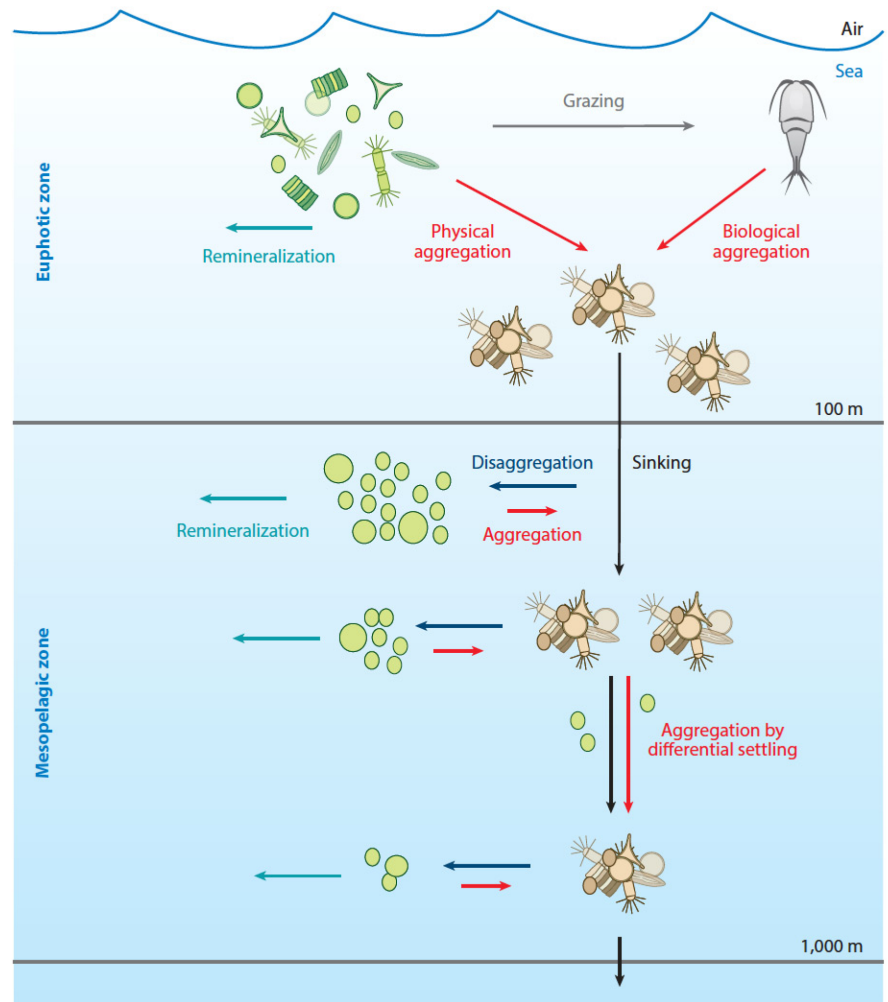


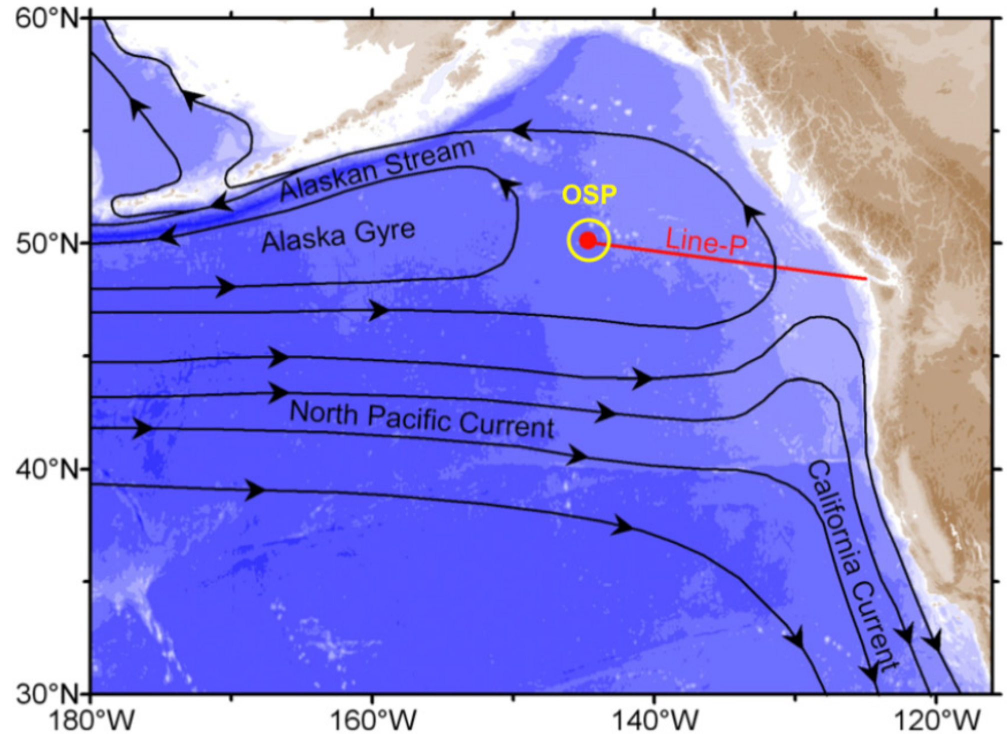
Figure from Lam & Marchal (2015)

The NASA EXPORTS North Pacific Cruise (summer 2018)

- 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)

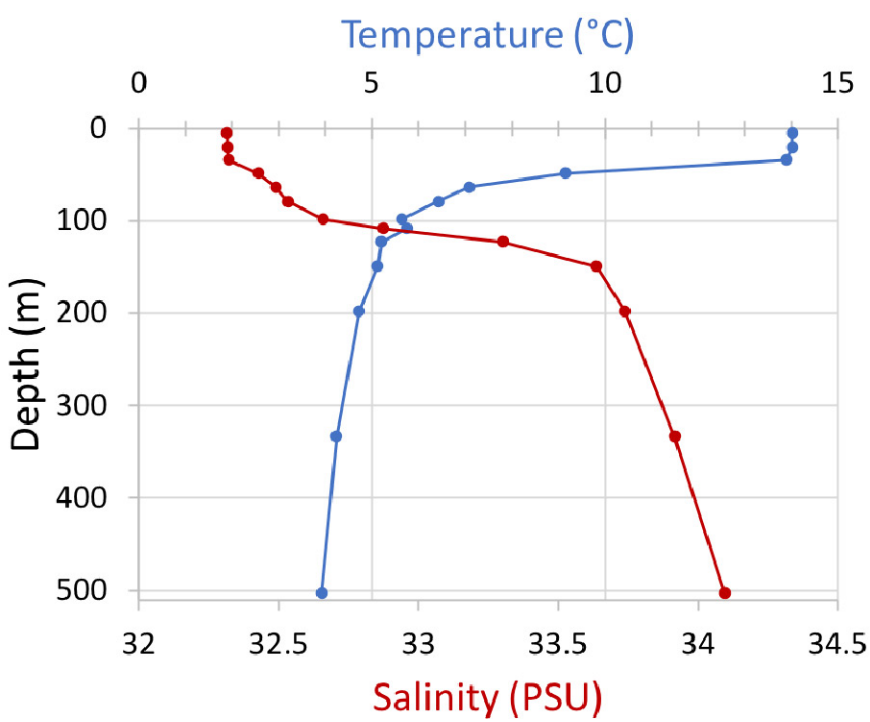
- Three size fractions collected, grouped into 2 size fractions for this study:
  - small size fraction, SSF (1-51 μm)
  - large size fraction, LSF (>51 μm)



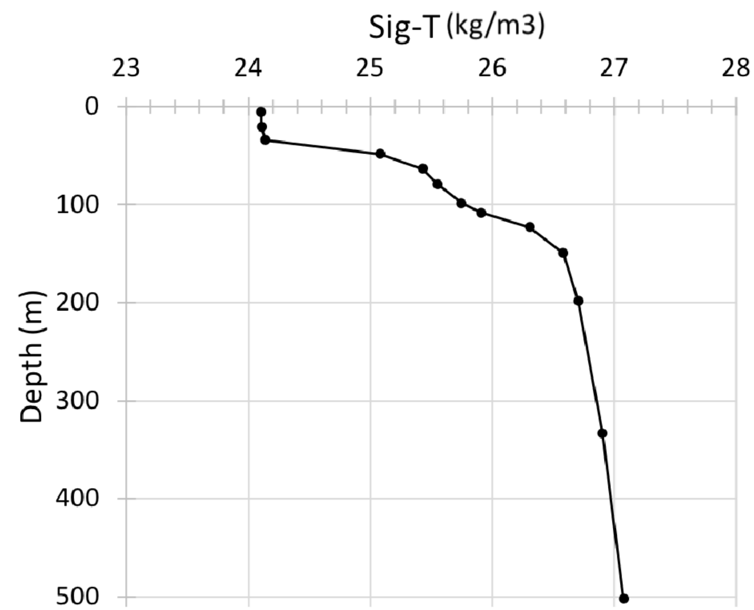
Map showing the location of Ocean Station Papa (OSP), the ship track (line P), and the major currents in the region. Modified from Freeland (2007).

OSP HYDROGRAPHY

- 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



Density (σ_T) profile 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)

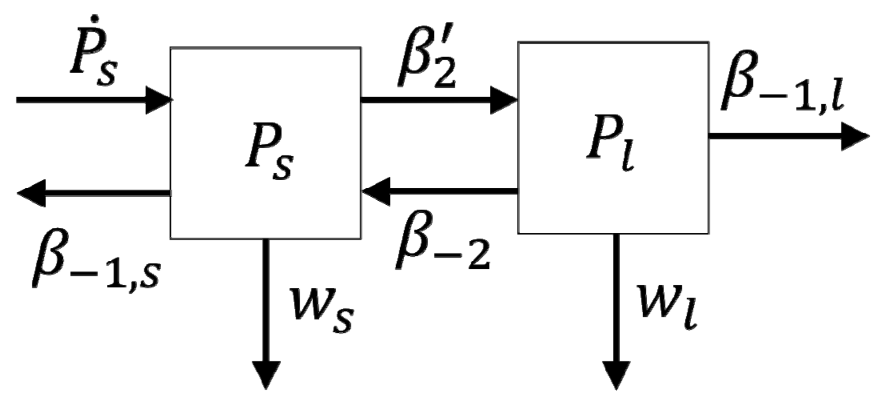
- Model grid: regular grid with $\Delta z = 5$ m

- Model assumptions:

  - steady state
  - one-dimensionality
  - all transport processes omitted except particle sinking
  - particle aggregation described with 2^{nd}-order kinetics
  - vertically uniform rate parameters except $\beta_{-1,s}$*

* rate constant for the remineralization of SSF particles

NUMERICAL MODEL OF POC CYCLING: schematic



<u>state variables</u>

P_s: [POC] in small size fraction (SSF)
P_l: [POC] in large size fraction (LSF)

<u>Parameters (r.c. = rate constant)</u>

$\dot{P}_s$:	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
β'_2:	r.c. for small particle aggregation
β_{-2}:	r.c. for large particle disaggregation

NUMERICAL MODEL OF POC CYCLING: balance equations

Small particles:

$$\underbrace{w_s \frac{dP_s}{dz}}_{\text{settling}} = \overbrace{\dot{P}_s}^{\text{production}} + \underbrace{\beta_{-2} P_l}_{\text{disaggregation}} - \overbrace{\beta_2' P_s^2}^{\text{aggregation}} - \underbrace{\beta_{-1,s} P_s}_{\text{remineralization}}$$

Large particles:

$$\underbrace{w_l \frac{dP_l}{dz}}_{\text{settling}} = \overbrace{\beta_2' P_s^2}^{\text{aggregation}} - \underbrace{\beta_{-2} P_l}_{\text{disaggregation}} - \overbrace{\beta_{-1,l} P_l}^{\text{remineralization}}$$

NUMERICAL MODEL OF POC CYCLING: treatment of particle production

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

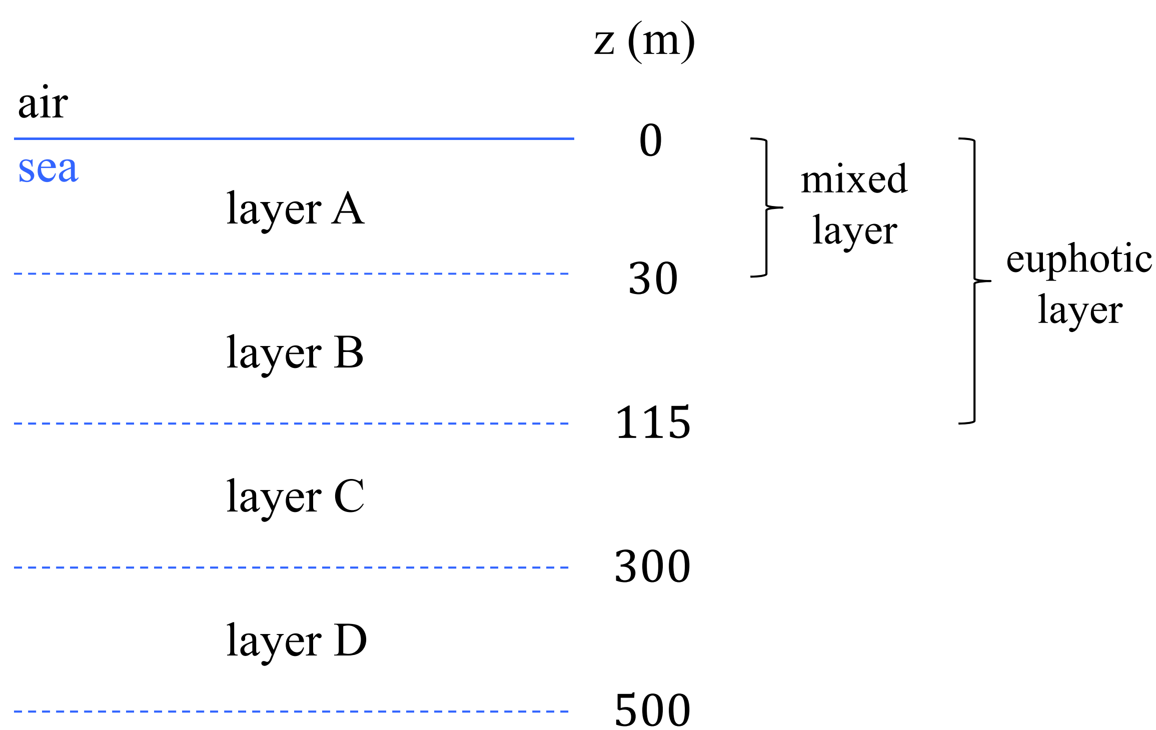
where

$\bar{\dot{P}}_s$	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)

NUMERICAL MODEL OF POC CYCLING: rate constants

- All rate constants of the model except the rate constant for the remineralization of small particles, $\beta_{-1,s}$, are assumed to be uniform in the upper 500 m.

- Motivated by independent evidence, the rate constant $\beta_{-1,s}$ is allowed to vary between four different layers in the upper 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

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

$$\text{where} \quad \begin{cases} \sigma_s^2 = \text{variance of POC data in SSF} \\ \sigma_l^2 = \text{variance of POC data in LSF} \\ L \;\; = \text{vertical covariance scale for POC} \end{cases}$$

UNKNOWNS OF THE INVERSE PROBLEM

- 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

$$\mathbf{x} = (w_s, w_l, \beta^A_{-1,s}, \beta^B_{-1,s}, \beta^C_{-1,s}, \beta^D_{-1,s}, \beta_{-1,l}, \beta'_2, \beta_{-2}, \bar{\dot{P}}_s, L_p, \overbrace{P_{s,1}, \dots}^{\text{95 values}}, \underbrace{P_{l,1}, \dots}_{\text{95 values}})^T$$

- The vector $\mathbf{x}$ 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).

STATEMENT OF THE INVERSE PROBLEM

- 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,

$$\boxed{J = (\mathbf{x} - \mathbf{x}_\mathrm{o})^\mathrm{T}\mathbf{C}_\mathrm{o}^{-1}(\mathbf{x} - \mathbf{x}_o) + \mathbf{f}(\mathbf{x})^\mathrm{T}\mathbf{C}_\mathrm{f}^{-1}\mathbf{f}(\mathbf{x})}$$

where

$\mathbf{x}_\mathrm{o}$	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
$\mathbf{C}_\mathrm{o}$	matrix containing the error (co)variances of the prior estimates in $\mathbf{x}_\mathrm{o}$
$\mathbf{C}_\mathrm{f}$	matrix containing the error (co)variances of the model equations

We assume $\mathbf{C}_f = \underbrace{\gamma}_{\text{trade-off parameter}} \mathbf{f}(\boldsymbol{x}_0)^{\boldsymbol{T}}\mathbf{f}(\boldsymbol{x}_0)\underbrace{\mathbf{I}}_{\text{identity matrix}}$

METHOD OF SOLUTION

- The inverse problem is nonlinear since some of the unknowns appear as products in the equations of the POC cycling model (consider, for example, $\beta_{-2}P_l$).

- 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 $\hat{\mathbf{x}}_k$, where k is the iteration step.

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

$$\boxed{\hat{\mathbf{x}}_{k+1} = \mathbf{x}_o + \mathbf{C}_o\mathbf{F}_k{}^T\left(\mathbf{F}_k\mathbf{C}_o\mathbf{F}_k{}^T + \mathbf{C}_f\right)^{-1}\left(\mathbf{F}_k[\hat{\mathbf{x}}_k - \mathbf{x}_o] - \mathbf{f}_k\right)}$$

where $\mathbf{F}_k$ = matrix of partial derivatives of $\mathbf{f}(\mathbf{x})$ with respect to $\mathbf{x}$ evaluated at $\mathbf{x} = \mathbf{x}_k$
$\mathbf{f}_k$ = vector of functions $\mathbf{f}(\mathbf{x})$ evaluated at $\mathbf{x} = \mathbf{x}_k$

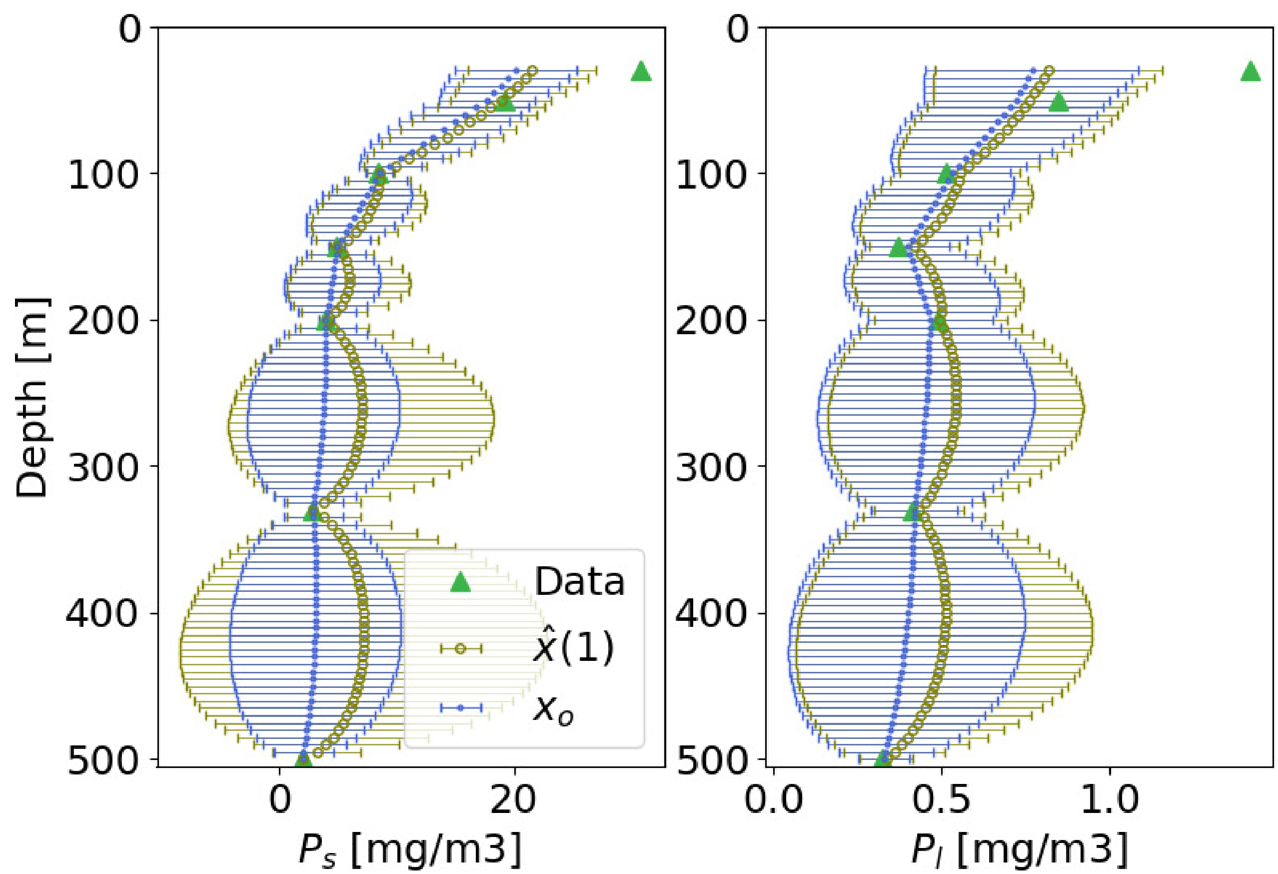
- The covariance matrix for $\hat{\boldsymbol{x}}_{k+1}$ is approximated from

$$\boxed{C_{k+1} = \left[\mathbf{I} - \mathbf{C}_o\mathbf{F}_k{}^T\left(\mathbf{F}_k\mathbf{C}_o\mathbf{F}_k{}^T + \mathbf{C}_f\right)^{-1}\mathbf{F}_k\right]\mathbf{C}_o\left[\mathbf{I} - \mathbf{C}_o\mathbf{F}_k{}^T\left(\mathbf{F}_k\mathbf{C}_o\mathbf{F}_k{}^T + \mathbf{C}_f\right)^{-1}\mathbf{F}_k\right]^T}$$

* *Tarantola & Valette* (1982)

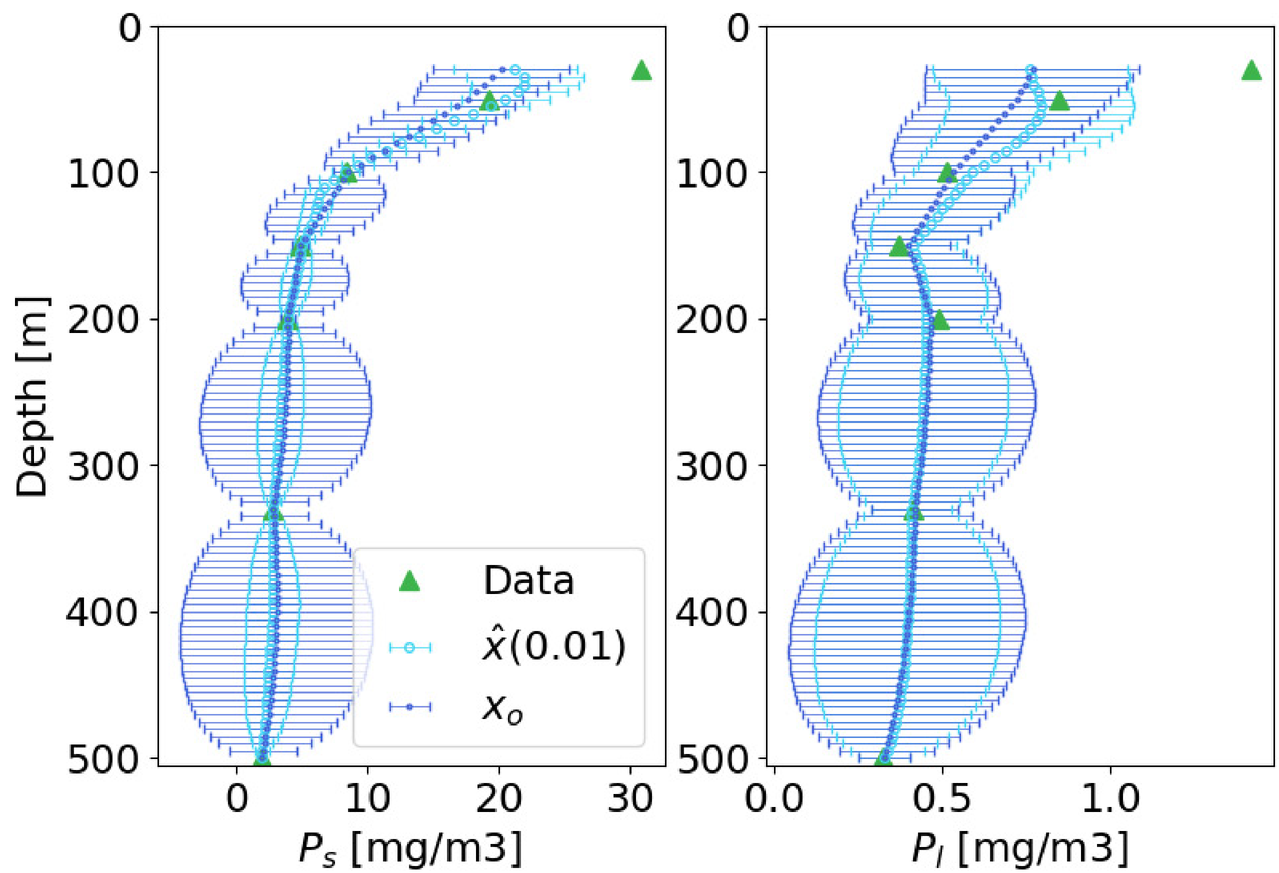
POC PROFILES ESTIMATED BY DATA INVERSION: solution with $\gamma = 1$

The solution with $\gamma = 1$ assumes a relatively low confidence in the POC cycling model.

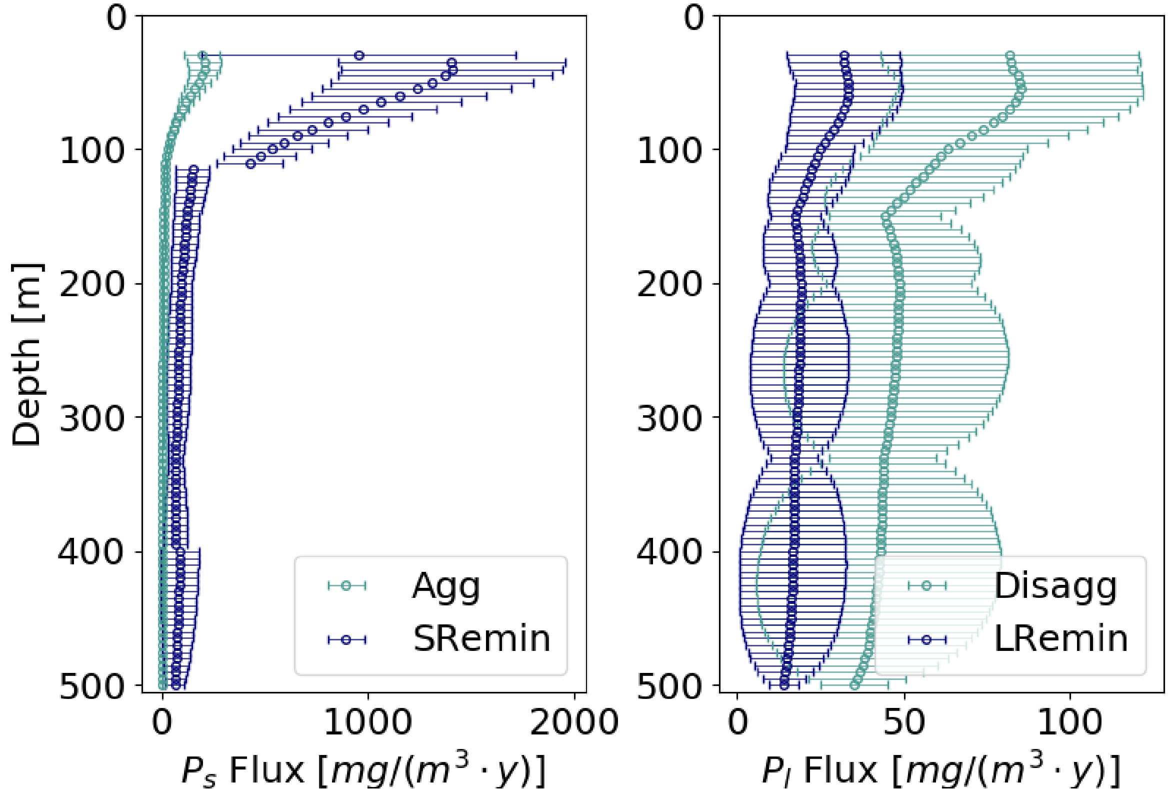


POC PROFILES ESTIMATED BY DATA INVERSION: solution with $\gamma = 0.01$

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.

REFERENCES

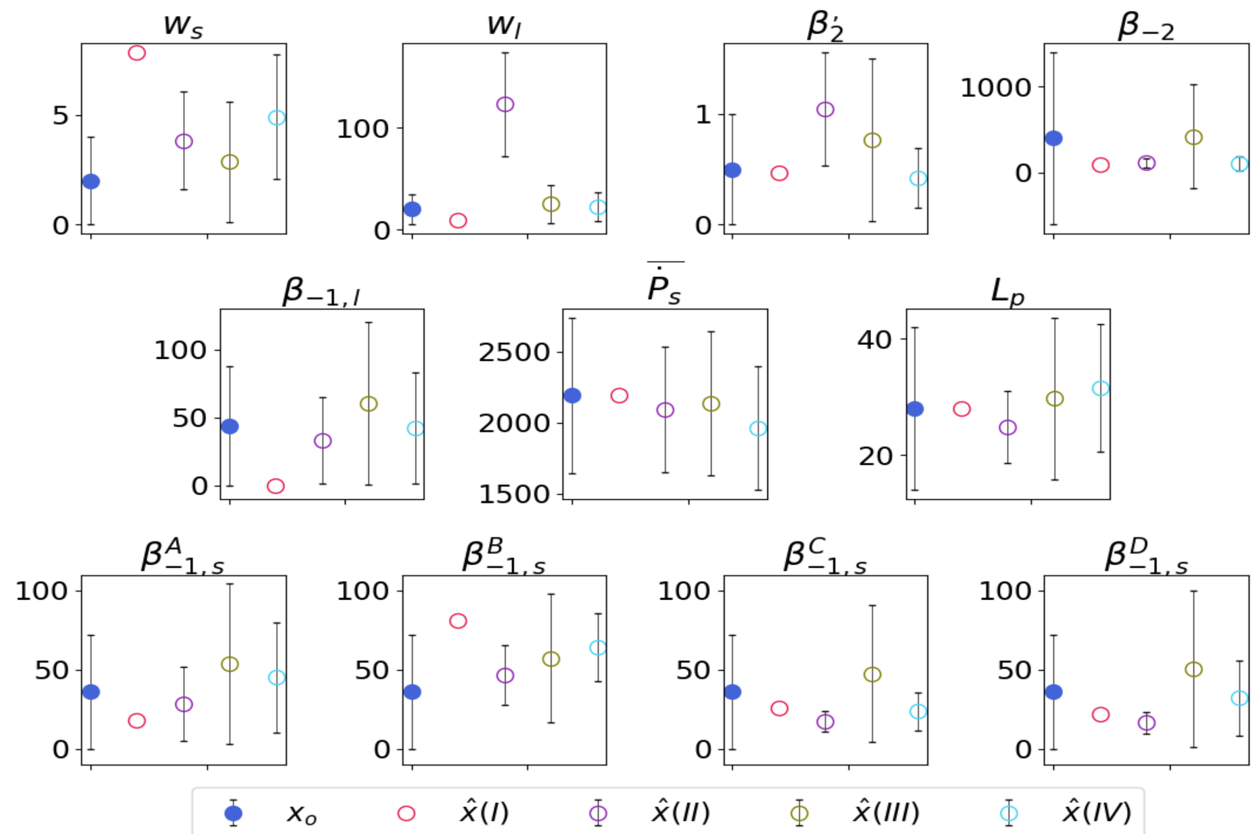
Freeland H., A short history of Ocean Station Papa and Line P, Progress in Oceanography, 75, 120–125, 2007

Lam P. and Marchal O., Insights into particle cycling from thorium and particle data, Annual Review of Marine Science, 7, 159-184, 2015

Tarantola A. and Valette B., Generalized nonlinear inverse problem solved using the least squares criterion. Reviews of Geophysics and Space Physics, 20, 219–232, 1982

BACK-UP SLIDE

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 ($\gamma = 0.01$)