Retrieval of phytoplankton pigments from underway spectrophotometry in the Fram Strait, Arctic Ocean

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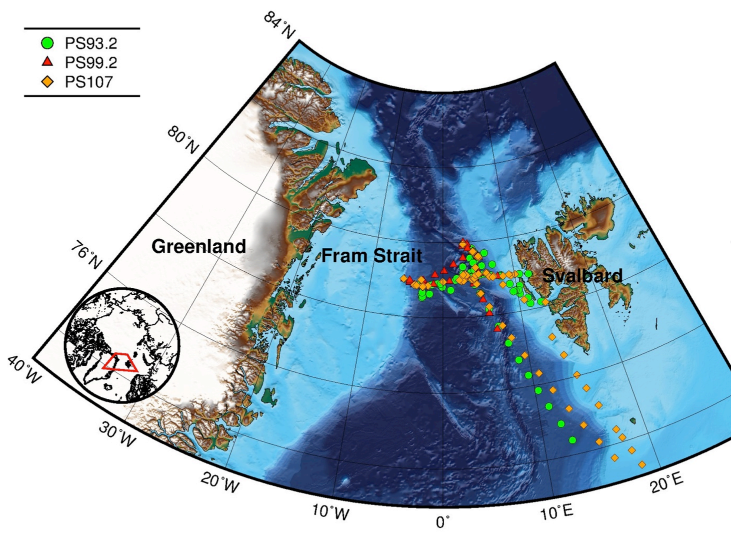
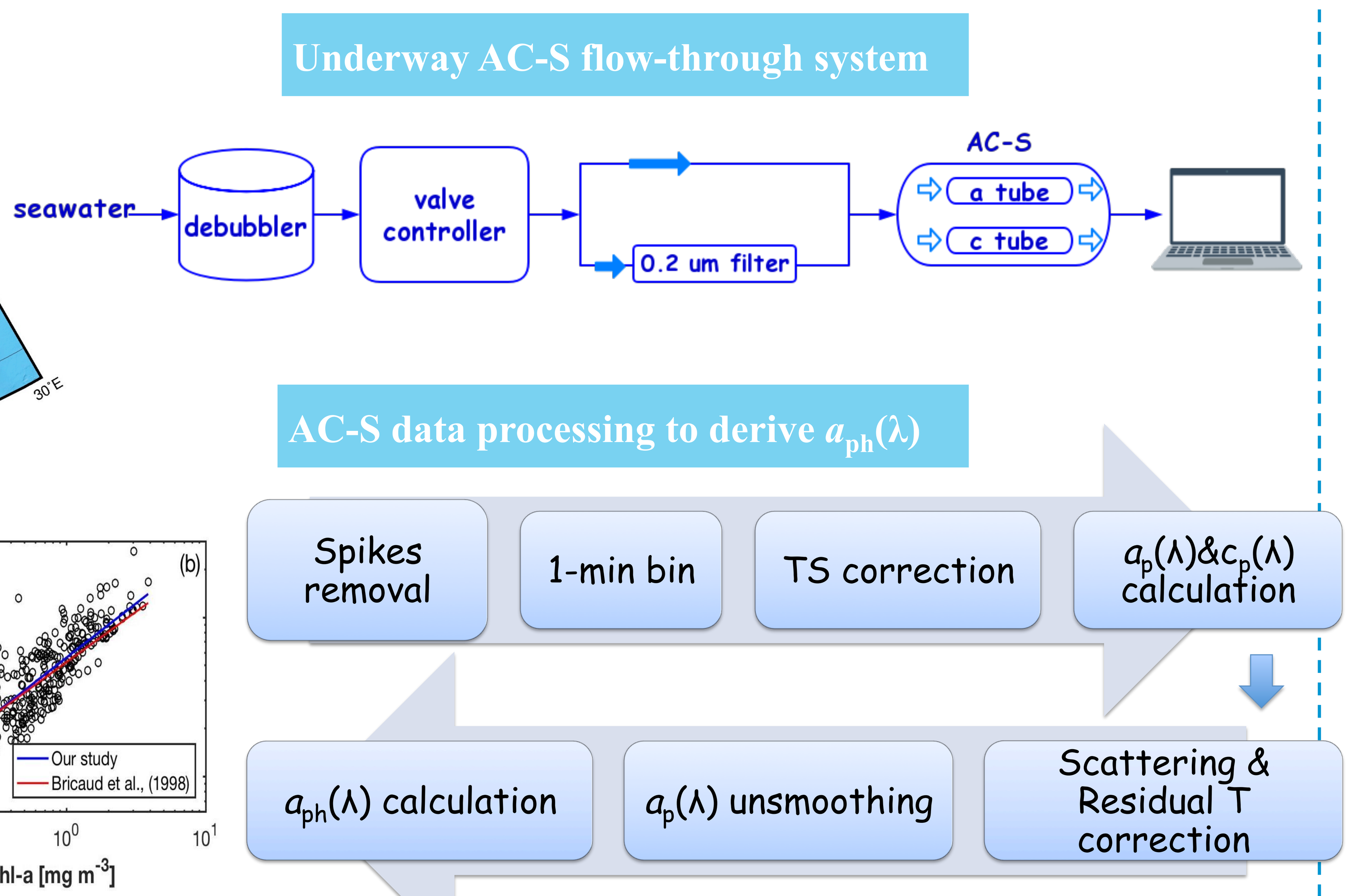
Introduction

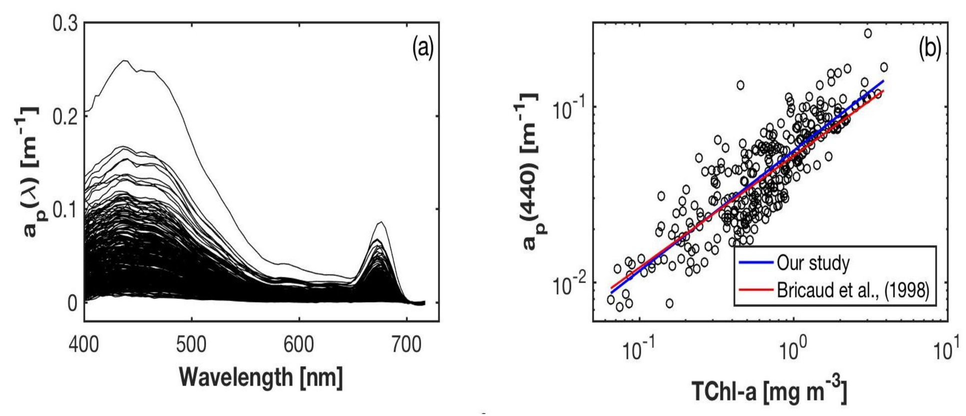
- ✓ Phytoplankton pigment databases have been extensively used in developing, validating or refining bio-optical algorithms for estimating phytoplankton biomass and functional types.
- ✓ Here, we investigate the performances of two approaches, i.e. Gaussian decomposition and singuar value decomposition combined with non-negative least squares (SVD-NNLS) in determining the concentrations of either individual pigments or pigment groups from $a_p(\lambda)$ obtained from underway AC-S flow-through system in the Fram Strait.
- ✓ The effect of package effect on the retrieval accuracy was assessed by including a normalization term in $a_{ph}(\lambda)$ (see below).

Data Collection & Processing

(Liu et al., 2018, and references therein)



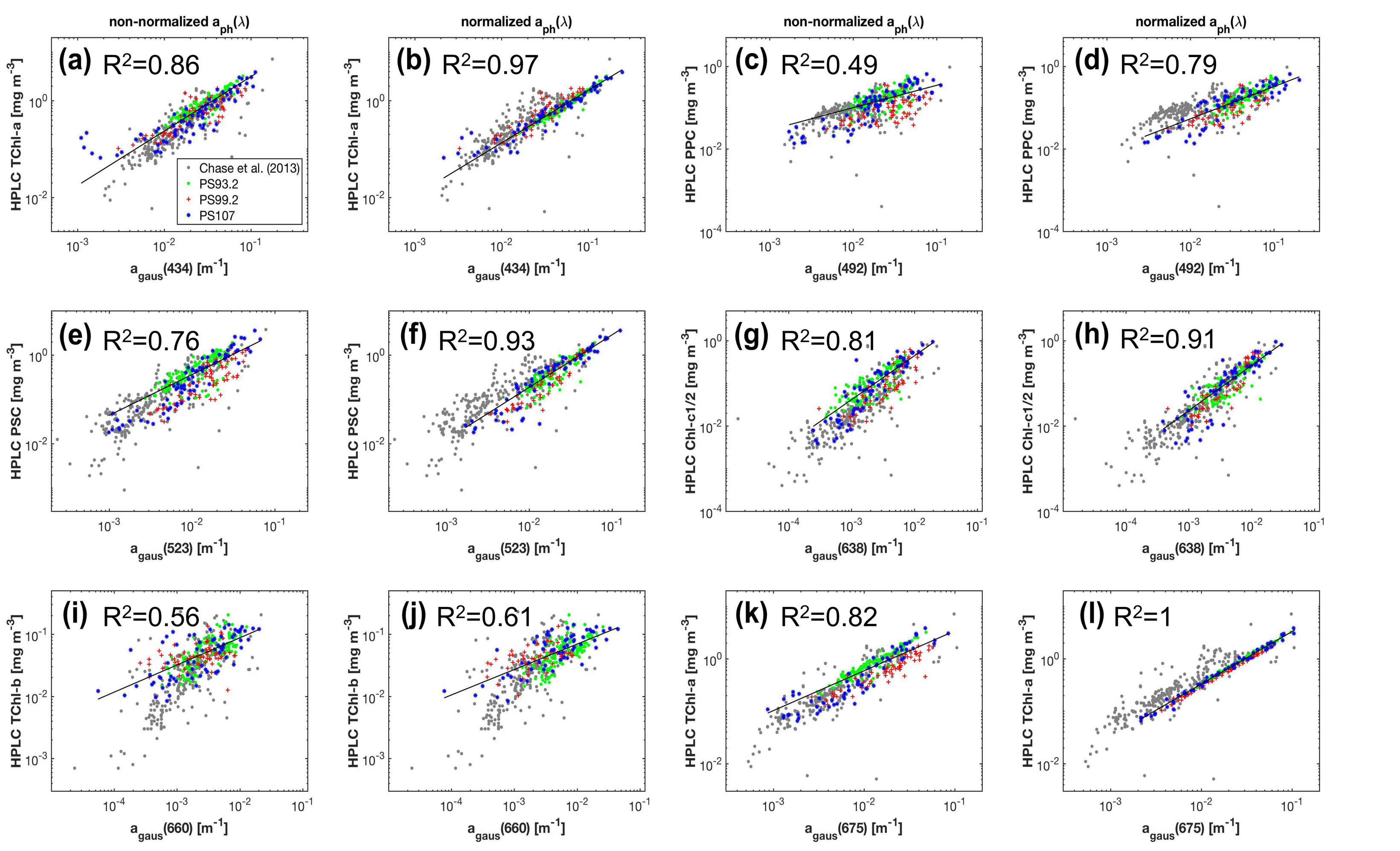




Gaussian Decomposition

(Chase et al., 2013)

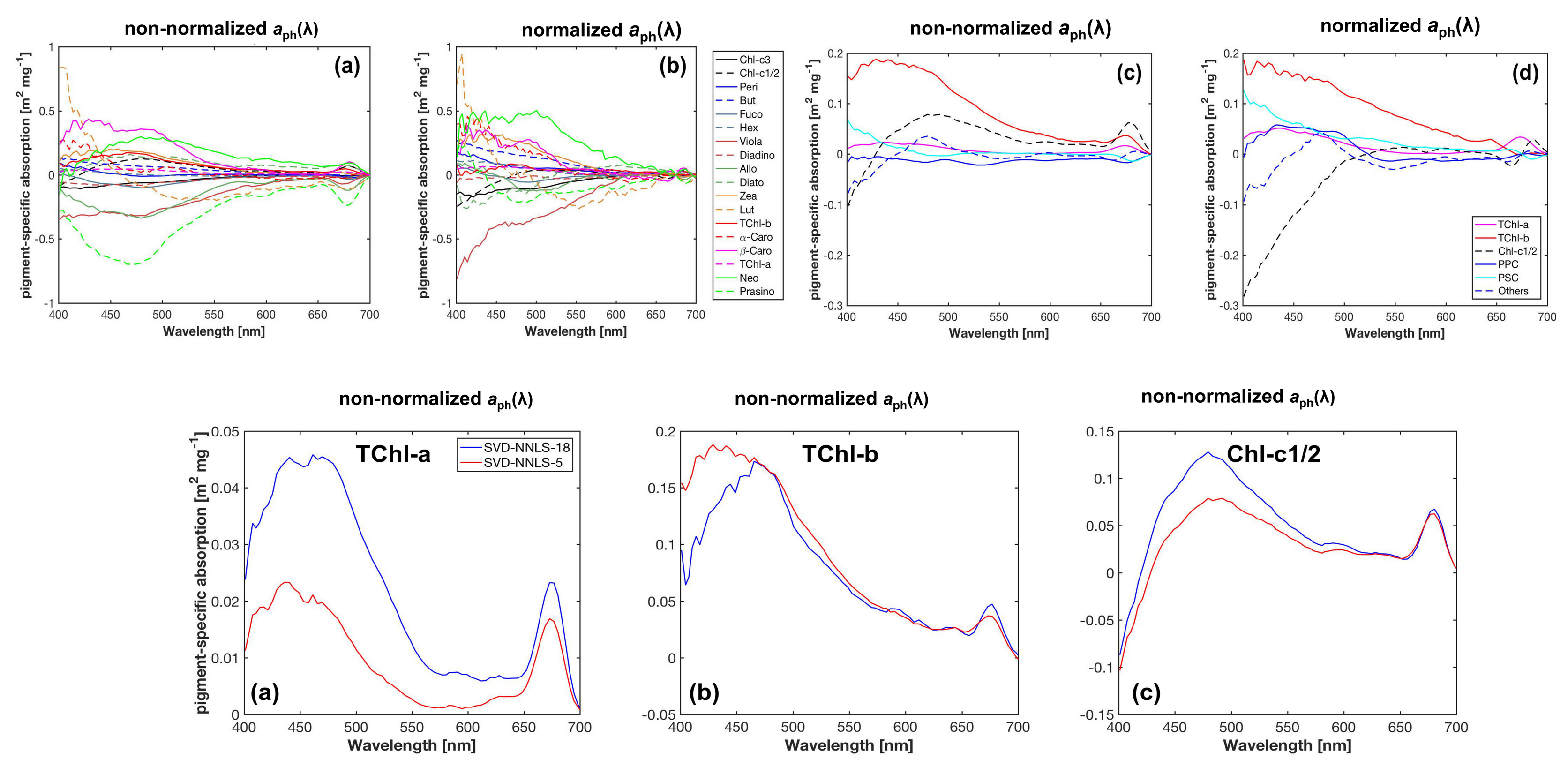
- ✓ $a_p(\lambda)$ was decomposed into 12 Gaussian functions + 1 NAP power law function.
- ✓ Gaussian amplitudes were related to the concentrations of TChl-a, TChl-b, Chl-c1/2, PSC and PPC.
- ✓ $a_{ph}(\lambda)$ normalized by package effect: $\hat{a}_{ph}(\lambda) = a_{ph}(\lambda)\dfrac{0.033 \times TChl-a}{a_{ph}(675)}$



SVD-NNLS

(Moisan et al., 2011)

- ✓ $a_{ph}(\lambda)$ can be reconstructed as $a_{ph}(\lambda) = \sum_{i=1}^{n} c_i a_i^*(\lambda)$
- ✓ In matrix form: 1) $C \cdot \tilde{A} = A_{ph}$ 2) $\tilde{A} \cdot \tilde{C} = A_{ph}$
- ✓ 1st inversion: pigment-specific absorption was solved using SVD.
- ✓ 2nd inversion: pigment concentration was solved using NNLS.
- ✓ SVD-NNLS-18: 18 types of pigments as input.
- ✓ SVD-NNLS-5: TChl-a, TChl-b, Chl-c1/2, PSC, PPC and the others as input.



Statistics (leave-one-out cross validation)

- ✓ relative percentage different (RPD). $RPD = \dfrac{1}{n}\sum_{i=1}^{n}\dfrac{C_i^{esti} - C_i^{meas}}{C_i^{meas}} \times 100\%$
- ✓ **bold**: pigments with better retrieval accuracy after applying the package effect normalization to $a_{ph}(\lambda)$.

Pigments	Gaussian Decomposition		SVD-NNLS-5		SVD-NNLS-18	
	non-normalized $a_{ph}(\lambda)$	normalized $a_{ph}(\lambda)$	non-normalized $a_{ph}(\lambda)$	normalized $a_{ph}(\lambda)$	non-normalized $a_{ph}(\lambda)$	normalized $a_{ph}(\lambda)$
TChl-a	11.9%	**2.3%**	6%	**-0.4%**	7.2%	**-0.2%**
TChl-b	15.3%	**12.0%**	53.3%	**39.1%**	93.8%	**88.8%**
Chlc_1/2	39.8%	**33.6%**	59.1%	63.1%	163.5%	170.5%
PSC	49.6%	**27.6%**	34.8%	44.5%	-	-
PPC	33.8%	**15.2%**	42.2%	**37.5%**	-	-
Chl_c3	-	-	-	-	280.2%	**202.6%**
Allo	-	-	-	-	28.2%	37.2%
α_Caro	-	-	-	-	102.0%	**71.2%**
β_Caro	-	-	-	-	51.0%	48.5%
Diadino	-	-	-	-	41.5%	47.3%
Diato	-	-	-	-	37.1%	60.2%
Fuco	-	-	-	-	56.0%	**49.8%**
Hex	-	-	-	-	67.1%	**51.5%**
But	-	-	-	-	249.1%	**97.2%**
Neo	-	-	-	-	14.8%	**12.3%**
Lut	-	-	-	-	29.4%	36.2%
Peri	-	-	-	-	64.1%	97.6%
Prasino	-	-	-	-	6.0%	**4.4%**
Viola	-	-	-	-	56.9%	71.0%
Zea	-	-	-	-	39.2%	39.7%
Others	-	-	49.5%	26.9%	-	-

Conclusion

- ✓ Gaussian decomposition was capable of estimating TChl-a, TChl-b, Chl-c1/2, PPC and PSC with a prediction error of less than 50% and outperformed SVD-NNLS in retrieving TChl-b, Chl-c1/2 and PPC.
- ✓ SVD-NNLS enabled the retrieval of a series of phytoplankton pigments with defined uncertainty (RPD ranges 6-280%).
- ✓ Lower uncertainties for the retrieval of all the five pigments using Gaussian decomposition and of 9 types of pigments using SVD-NNLS were obtained with the combined use of observed $a_{ph}(\lambda)$ and TChl-a concentration that partially accounts for the package effect across the whole absorption spectra.

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