Stability of Physically Modeled versus Data-Extracted End-Members for Multispectral Decomposition of Coastal Water Reflectance

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Sharing is encouraged

1- Background

- Coastal waters (Case-II) are **optically complex**
- Multiple constituents affect surface reflectance:
  - Chlorophyll-*a* (Chl*a*)
  - Total Suspended Matter (TSM)
  - Colored Dissolved Organic Matter (CDOM)
- Existing approaches:
  - Empirical → site-dependent
  - Analytical → complex & sensitive
  - Machine Learning → black-box
- **Key Challenge**:
  Separating mixed spectral signals into physically meaningful components

2- Objective

Develop a physically interpretable and scalable framework to:

- ✓ Decompose reflectance spectra using Gaussian Spectral Decomposition (GSD)
- ✓ Extract constituent-related features
- ✓ Retrieve Chl*a* & TSM accurately
- ✓ Work for both *in-situ* & satellite data

3- Study Area & Data

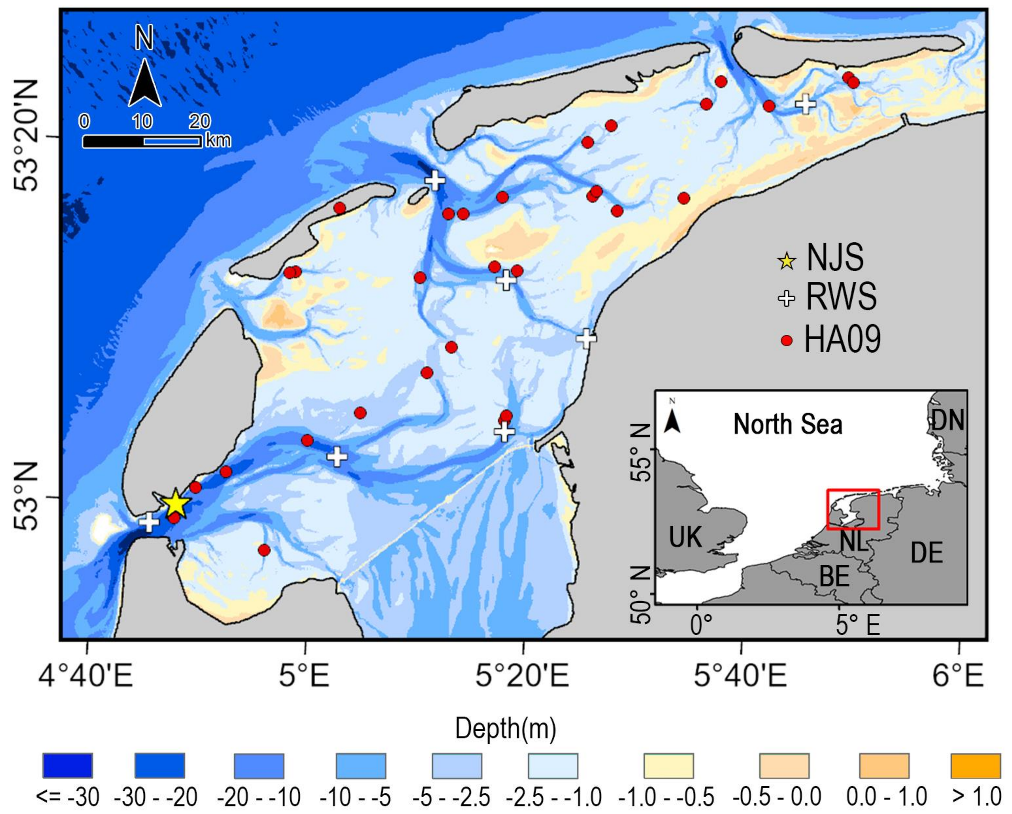
Dutch Wadden Sea (Highly turbid coastal system)

Datasets:

- *In-situ* hyperspectral *Rrs*(λ)
- *In-situ* Chl*a*, TSM, and CDOM
- Long-term water quality measurements

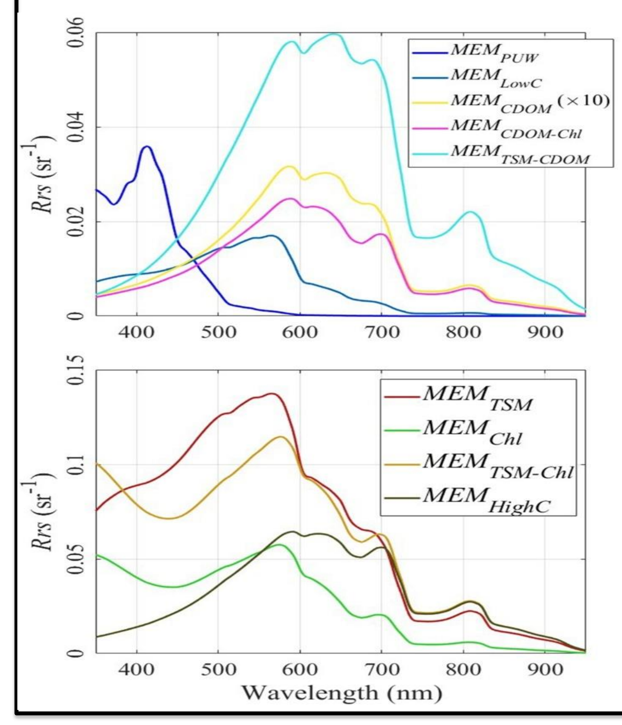
Satellite:

- Sentinel-2 MSI
- Sentinel-3 OLCI



4- Methodology

- Bio-optical modeling → Modeled End-Members
- *In-Situ* / Satellite observation → Extracted End-Members (*EE* algorithm)
- Gaussian Spectral Decomposition
- Spectral Gaussian Parameters amplitude (*A*), central wavelength (*μ*), bandwidth (σ)
- Construct Gaussian basis library
- Measured *in-situ*/satellite $R_{rs}(\lambda)$
- FCLSU spectral unmixing
- Aggregate Gaussian Coefficients
- End-member abundances
- Predict Chl*a* and TSM (Random-Forest model)



The modeled end-members (*MEMs*) generated from the combinations of Water constituents Concentrations (WCCs)

6- Key Results & Conclusion

- **In-situ Retrieval Performance**
  - Stable across *MEMs* & *EEMs*

Parameter	R^2	RMSE
TSM	~0.73–0.74	~6.3 g/m³
Chla	~0.79–0.81	~4.0 mg/m³

- **Satellite Retrieval (Key Insight)**
  - ***MEMs* outperform *EEMs***
  - More robust to:
    - ✓ Noise
    - ✓ Atmospheric correction
    - ✓ Spectral Band limitations

Sensor	Parameter	R^2 (MEMs)	R^2 (EEMs)
S2-MSI	TSM	0.64	0.57
S3-OLCI	TSM	0.69	0.59
S2-MSI	Chla	0.78	0.63
S3-OLCI	Chla	0.73	0.65

Conclusion

- GSD enables **accurate + interpretable** WCC retrieval
- MEMs are:
  - ✓ More stable
  - ✓ More transferable
  - ✓ Less sensitive to noise

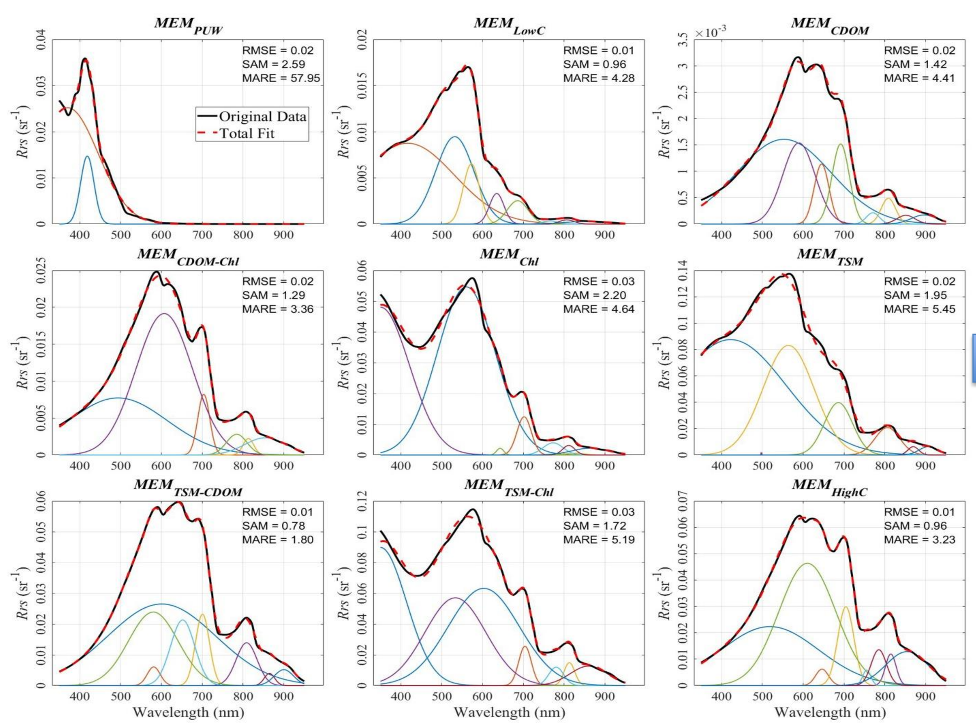
GSD is Suitable for **operational coastal monitoring**

Sharing is encouraged

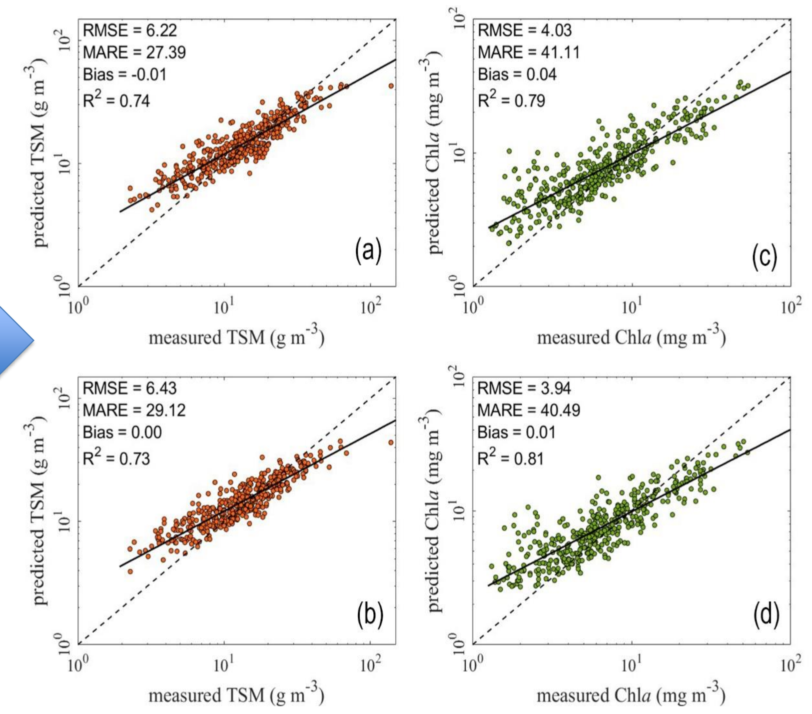
The MATLAB code for Gaussian Spectral Decomposition can be accesses at **https://github.com/arminaMMX/GSD_for_Water_Quality**

5- Results

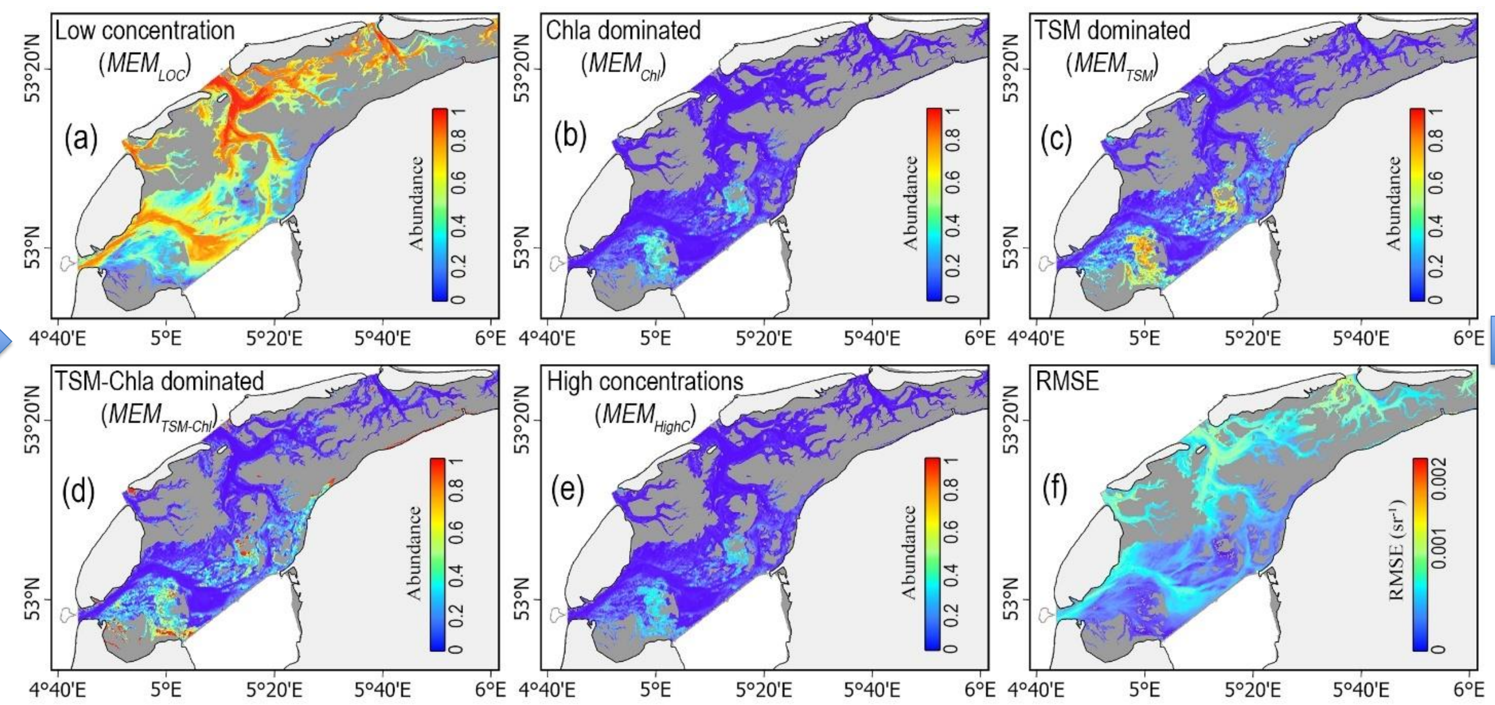
Spectral decomposition of *MEMs* into Gaussian components.



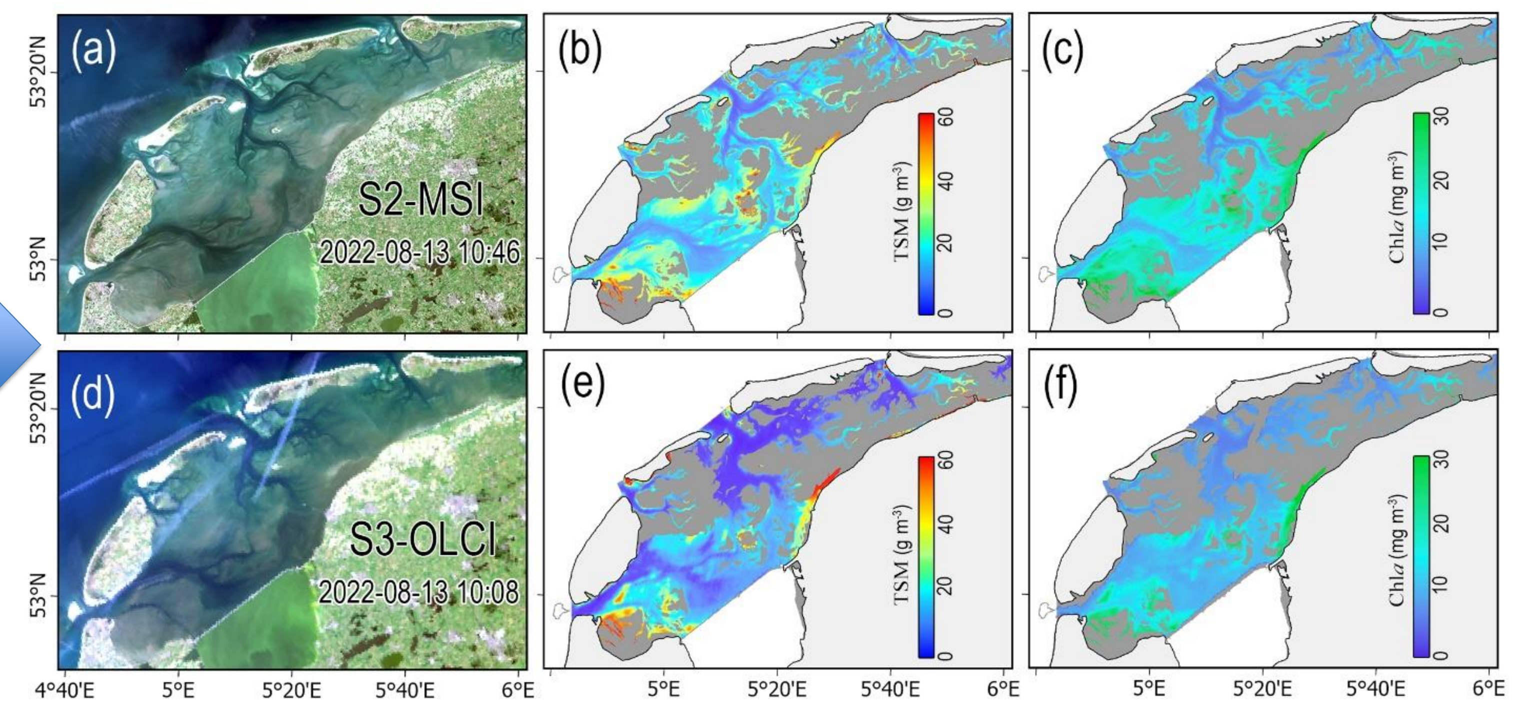
Correlation between measured and predicted WCCs

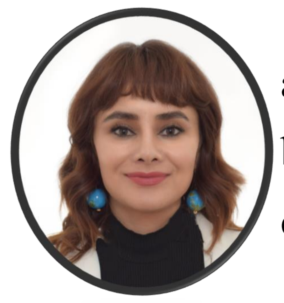


Abundance maps of the five *MEMs* fractions derived from S2-MSI *Rrs*(λ) spectra using GSD



Application of the GSD model to S2-MSI and S3-OLCI imageries





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