ARIS

14th Annual SABCS Workshop

Vancouver, BC

25 September 2024

Development of a Light Absorption Model for Phototoxic PAHs

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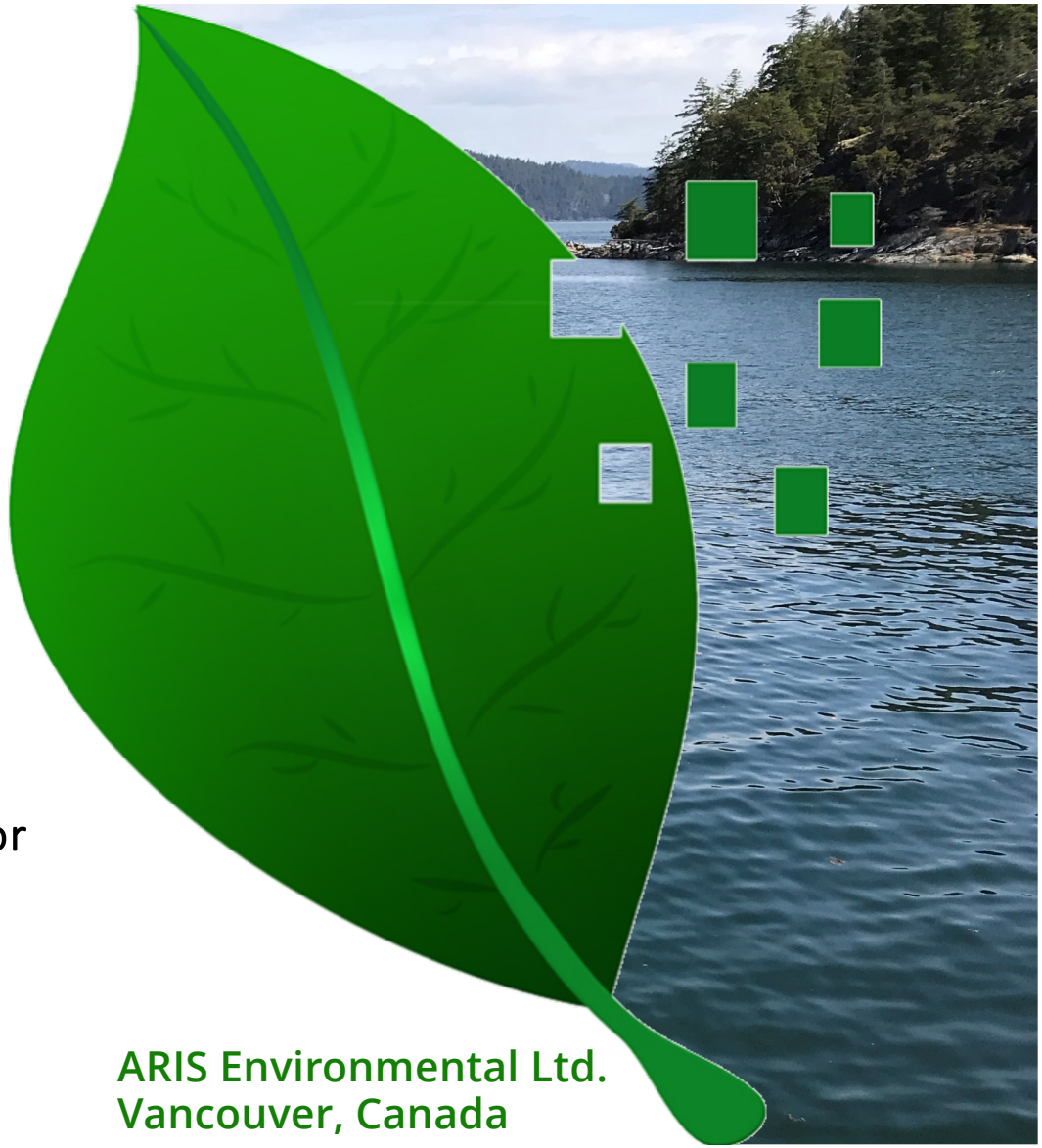


ARIS Environmental Ltd.
Vancouver, Canada

Acknowledgements

- Angeline Tillmanns (BC WLRS)
- Sasha Madronich (NCAR)

  US National Center for Atmospheric Research
- Jasen Nelson (BC ENV)
- Canadian Council of the Ministers of the Environment PAH Project Team, including:

  Allison Dunn (ECCC)

  Angeline Tillmanns (BC WLRS)

  Janet Cermak (ECCC)

  Yves Rochon (ECCC)

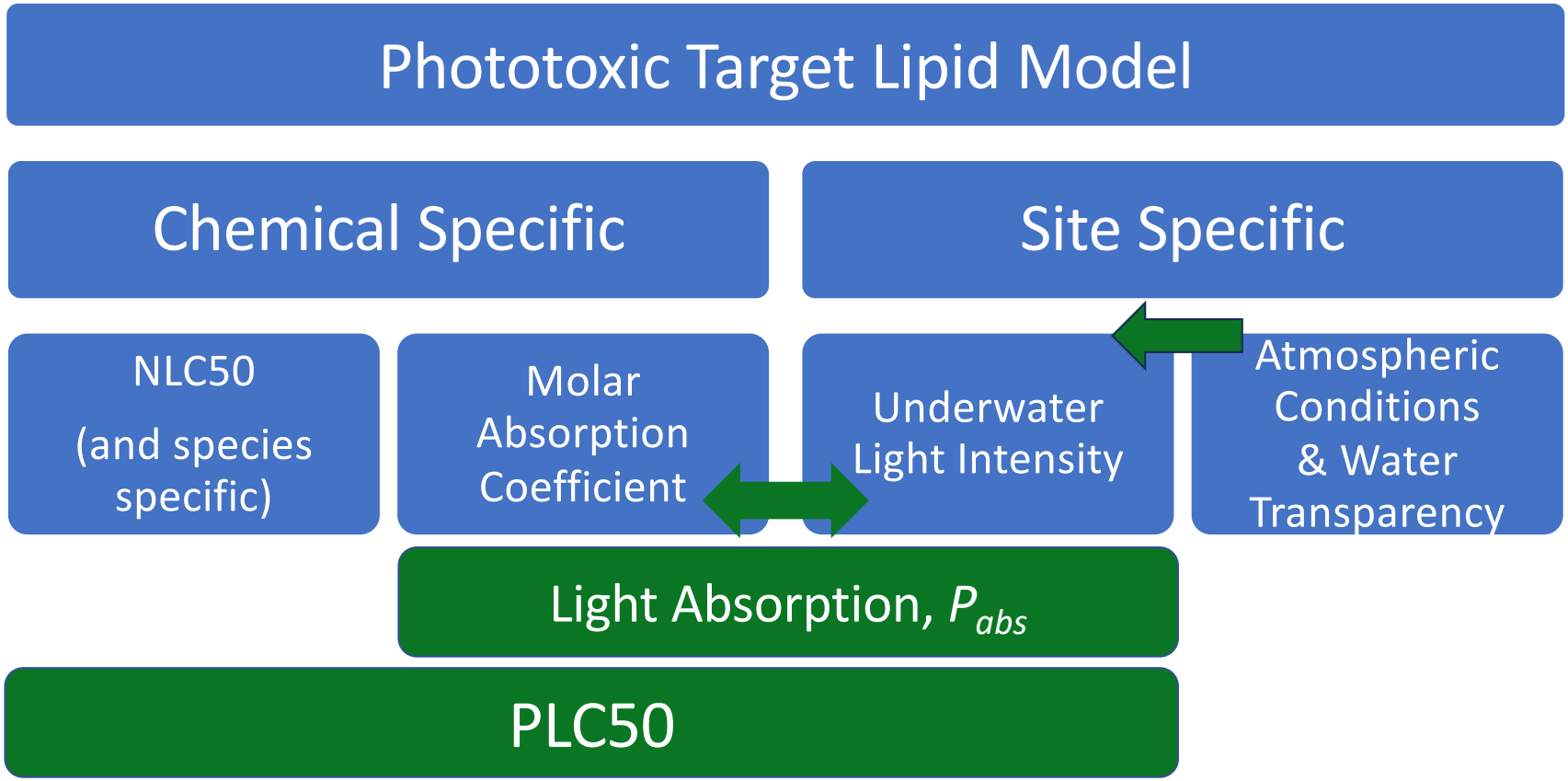
Water Quality Guidelines for Phototoxic PAHs

Empirical Model

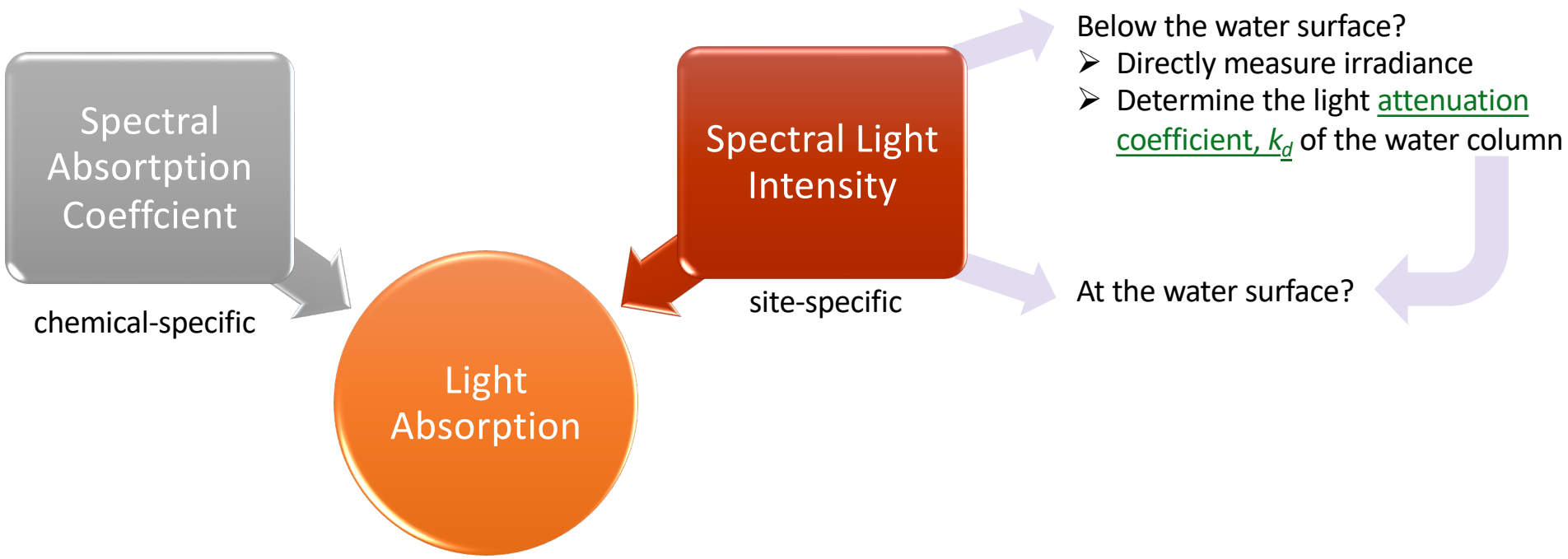
(target lipid model)

Site-Specific Light Absorption Model

Water Quality Guidelines for Phototoxic PAHs



Problem Formulation



Proposed Solution

Modified Tropospheric Ultraviolet and Visible (TUV) model

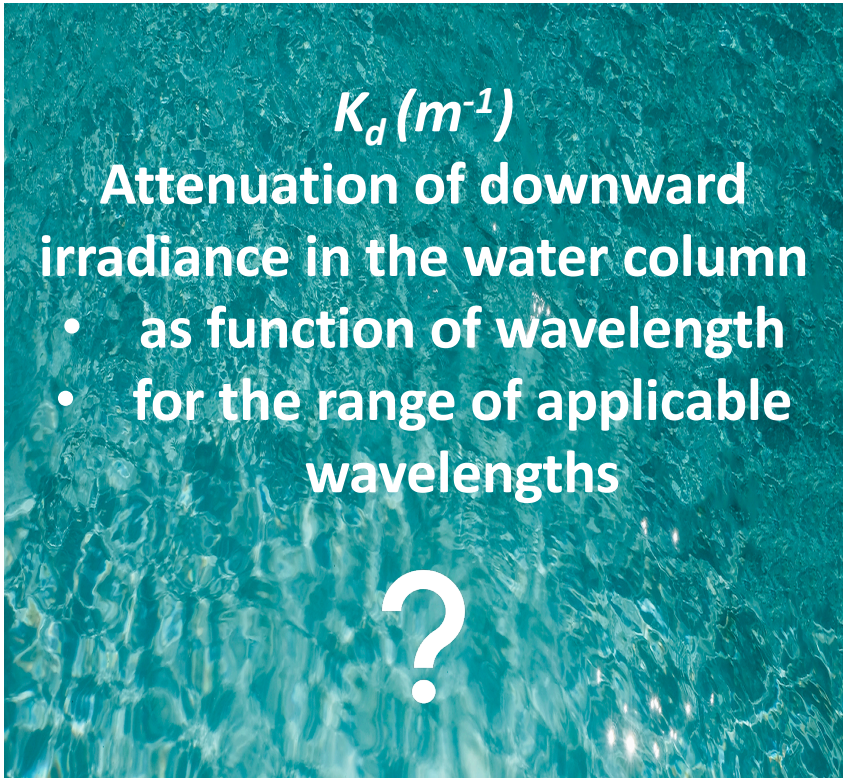
Solar position ✅
- Location
- Date & time

Atmospheric conditions ✅
- Cloud cover
- Ozone column
- Aerosols

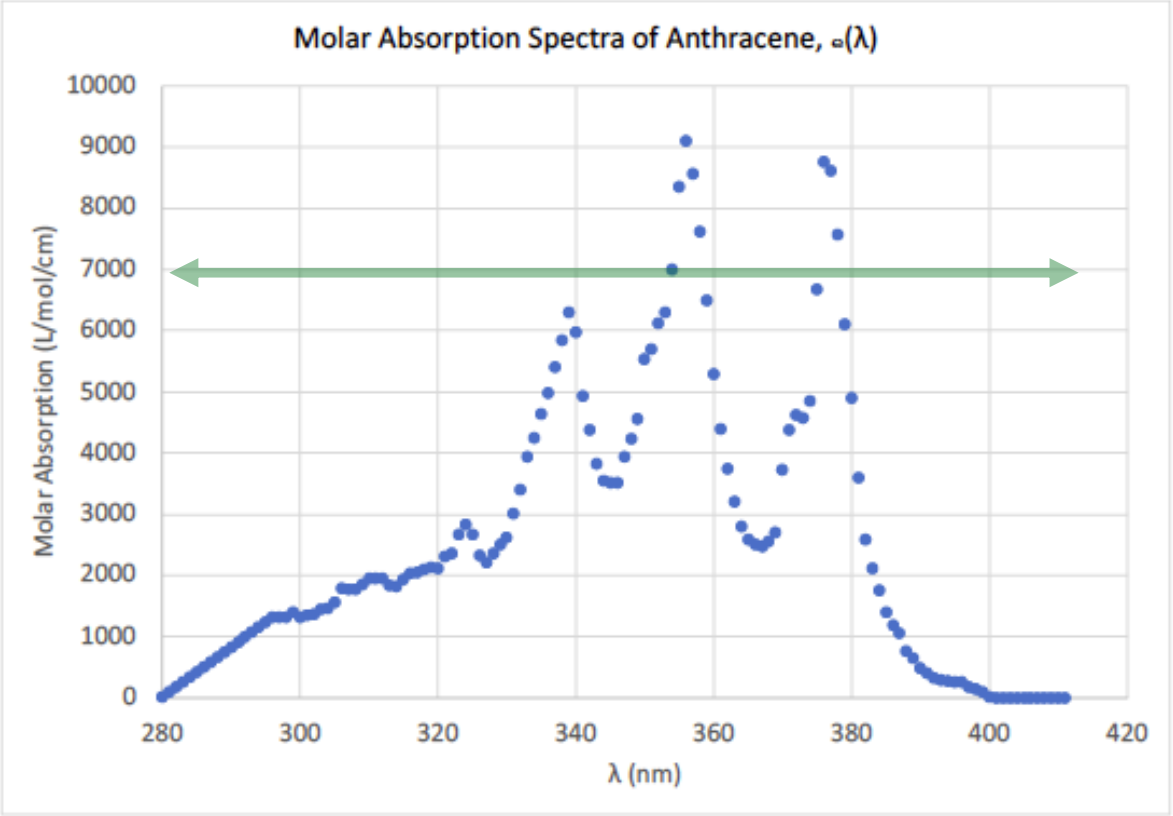
Water surface albedo ✅

Water depth ✅

Exposure duration ✅



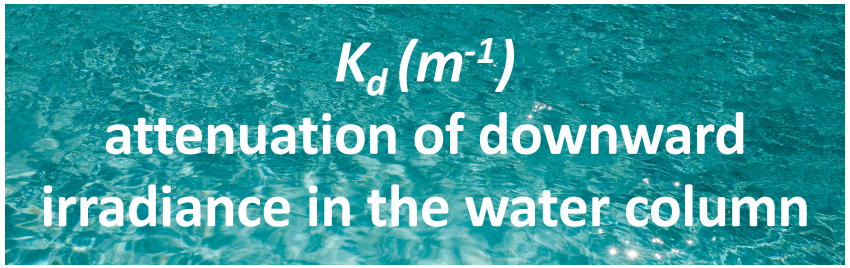
Example Molar Absorption Spectra



Includes UVA/UVB range

Light Attenuation Coefficient?

1. Measurements of downward irradiance using a radiometer (vertical profile) and exponential fit to the irradiance versus depth (Beer-Lambert expression)
2. Remote sensing satellite data of reflectance
3. ✅ Estimated from the inherent optical properties (IOPs) related to the light absorbing & scattering components (or water quality parameters)



Results of the Literature Search - Summary

- Freshwater & Marine Environments
- Freshwater k_d model at reference wavelength (305 nm)

$$k_{d,305} = a_{305}[DOC]^{b_{305}} + k_{water}$$

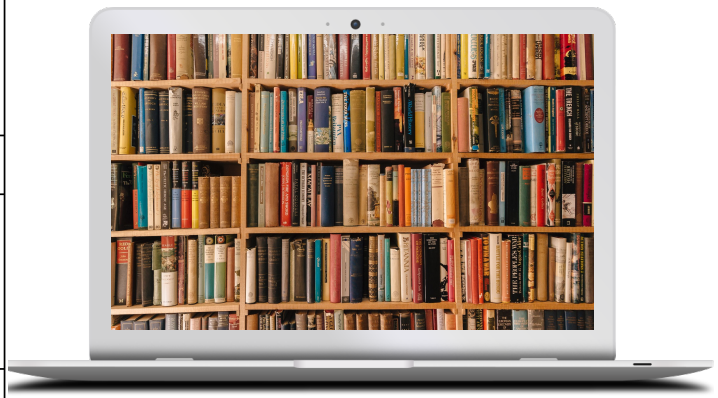
- Spectral k_d model (marine and freshwater)

$$k_d(\lambda) = k_{d,305}e^{S_k(305-\lambda)}$$

- Freshwater model validation
- Marine k_d model

Data Compilation – Freshwater Environment

Study	DOC Range (mg/L)	k_d wavelength Or waveband (nm)	CHL-a (mg/m³)	TSS* (g/m³)	Number of locations	Paired DOC-k_d data	Use
Morris et al (1995) Lakes in Alaska, Colorado, Pennsylvania, and Argentina	0.24 – 23.5	305	0 – 5.1	0.02 – 7.36 (PM)	45	45	MD & CV
		320				64	V
		340				64	
		380				63	
V.-Balogh et al (2009) Shallow lakes and ponds in Hungary	1.21 – 61.45	305	1.45 – 152.96	0.96 – 188.53 (TSS-Alg)	30	30	MD & CV
		313				30	V
		320				30	
		340				30	
		380				30	
		395				30	
Smith et al (2004) Laurentian Great Lakes and tributary rivers	2.43 – 8.00	305	0.85 – 13.1	0.78 – 4.56	6	6	MD & CV
		325				6	V
		340				6	
		380				6	



10 studies
877 paired DOC – k_d data points
173 locations

Model Development & Validation

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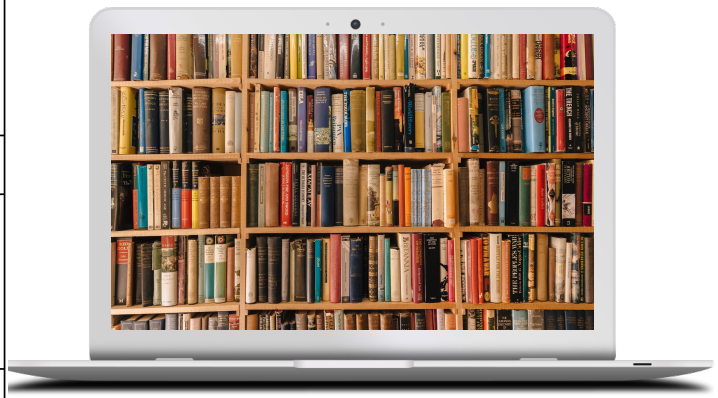


model development & cross validation (MD & CV)
3 studies, 81 datapoints

In-sample & out-of-sample validation (V)
10 studies, 877 datapoints

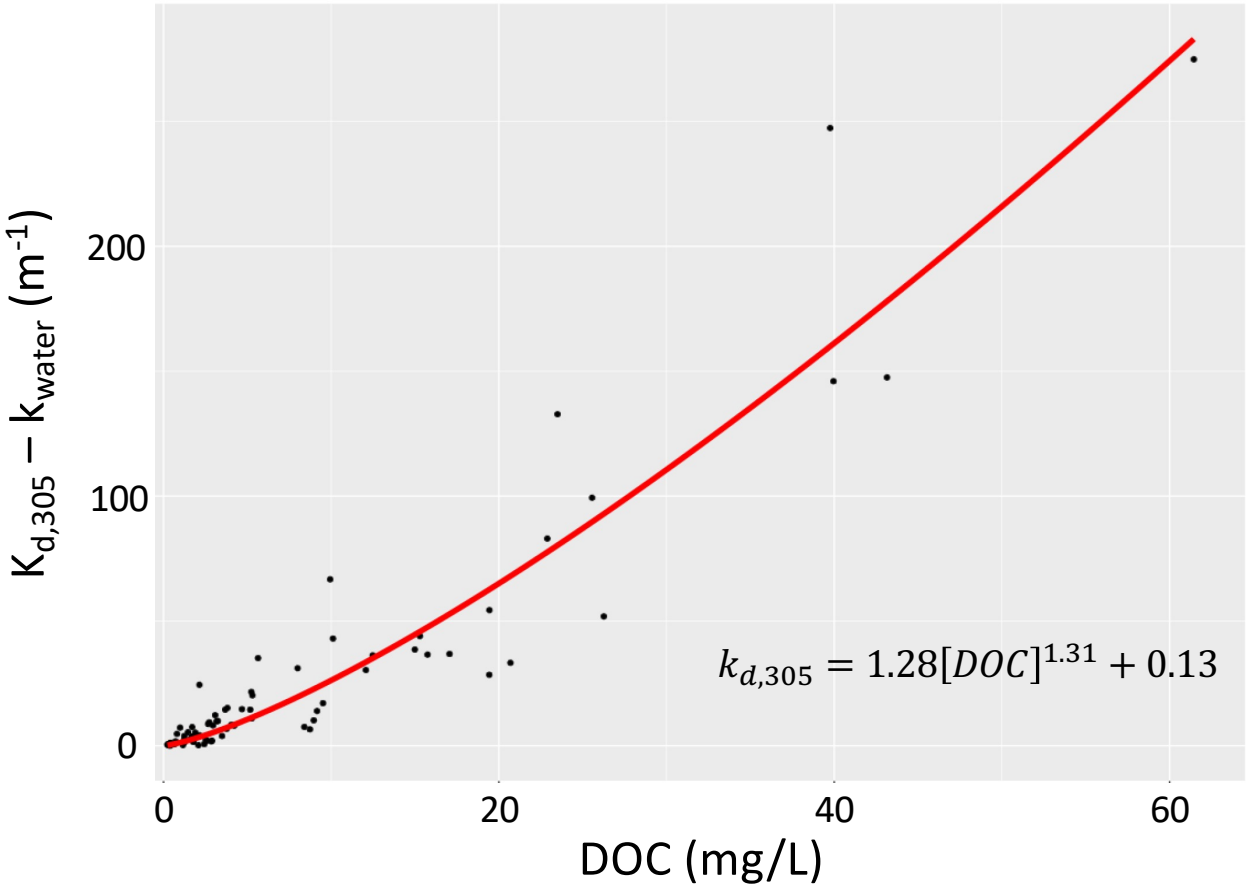
New Model with Combined Dataset

- Predicted light absorption sensitive to k_d ⇒ new model with expanded dataset

Model	Morris et al (1995) Study	All Data Combined
Number of data points	45	81
Standard deviation on k_d data	22.5	48.8
Residual Standard Error	4.65	16.17
a_{305}	2.67	1.28
b_{305}	1.25	1.31

Least-squares nonlinear fitting procedure

Power Law Model for Reference Wavelength



Cross Validation Results

- Leave-one-out cross validation (LOOCV) method

Model	Morris et al (1995) Study	All Data Combined
Number of data points	45	81
Standard deviation on k_d data	22.5	48.8
Root Mean Square Error (RMSE)	5.59	17.14
R^2	0.946	0.875
Mean Absolute Error (MAE)	3.01	8.65

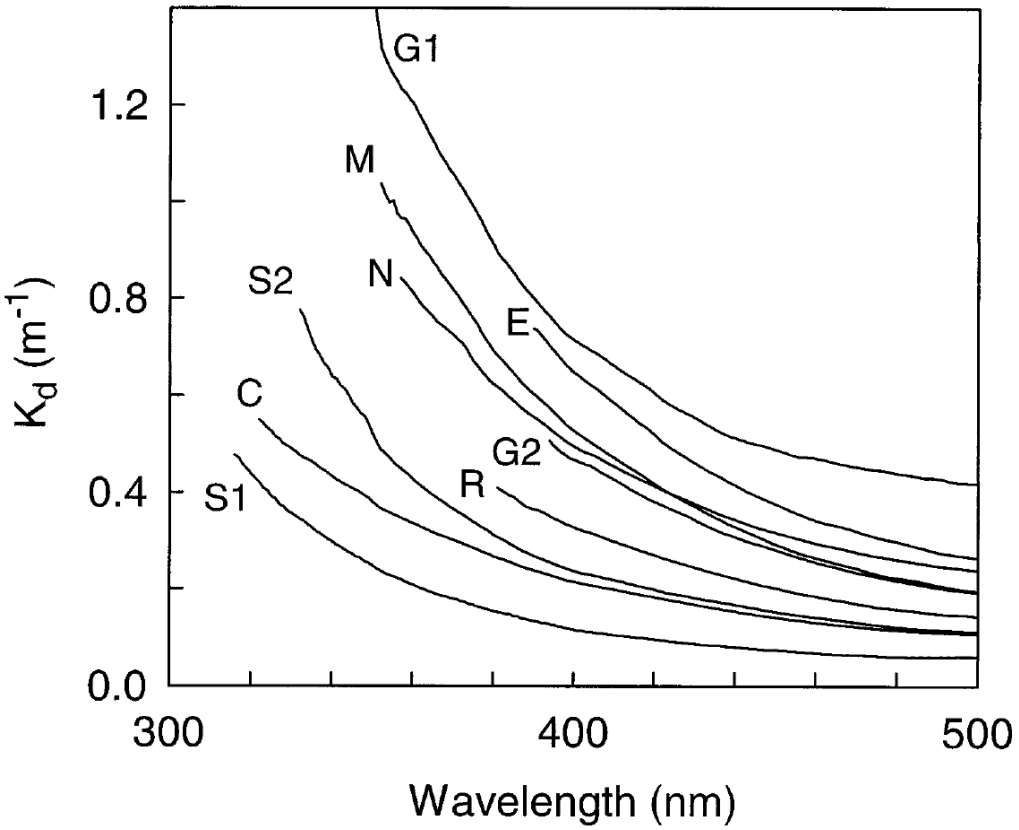
- Effect of other water quality parameters
- Model to data ratio
  - Various wavelengths
  - In-sample and out-of sample (877 paired data points)

Additional Model Comparison

- Effect of other water quality parameters
- Model to data ratio
  - Various wavelengths
  - In-sample and out-of sample (877 paired data points)

Model	Model : Data > 2	Model : Data < 0.5	Model : Data > 10	% over-estimated by factor > 2
Morris et al (1995) dataset	256	25	6	29
Combined model (81)	69	198	0	8

Spectral k_d Values



Markager & Vincent (2000)

7 lakes in high arctic Canada
& literature review

$$k_d(\lambda) = k_{d,305} e^{S_k(305-\lambda)} + k_{back}$$

Marine k_d Model

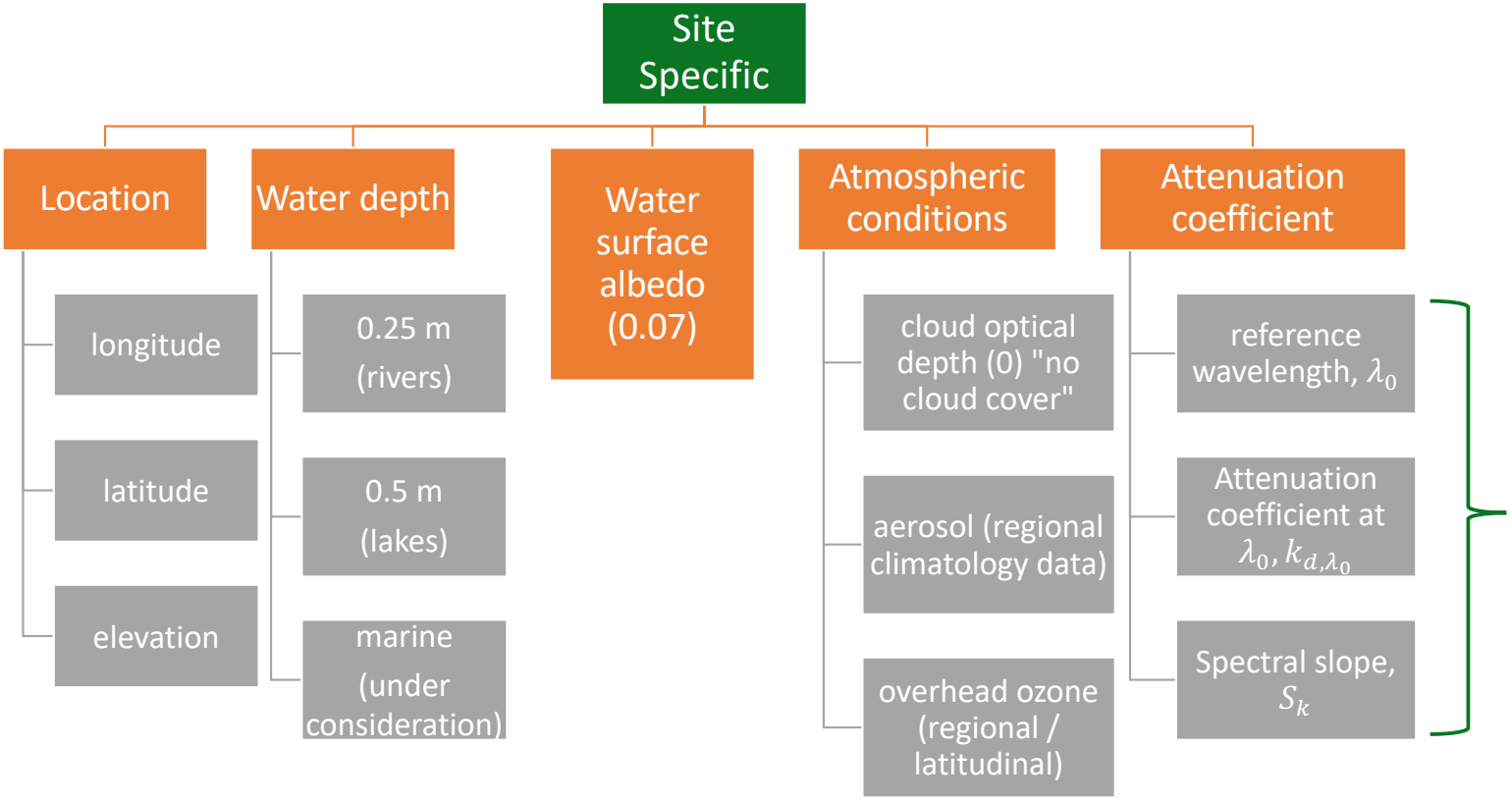
- Function of CHL concentration (literature search and data analysis)
- Applicable depth is low -> limited attenuation expected
- Non-site specific default value:

$$k_{d,305} = 1.4 \text{ m}^{-1}$$

- Spectral k_d model (marine)

$$k_d(\lambda) = k_{d,305} e^{S_k(305-\lambda)} \; ; \; S_k = 0.014 \text{ nm}^{-1}$$

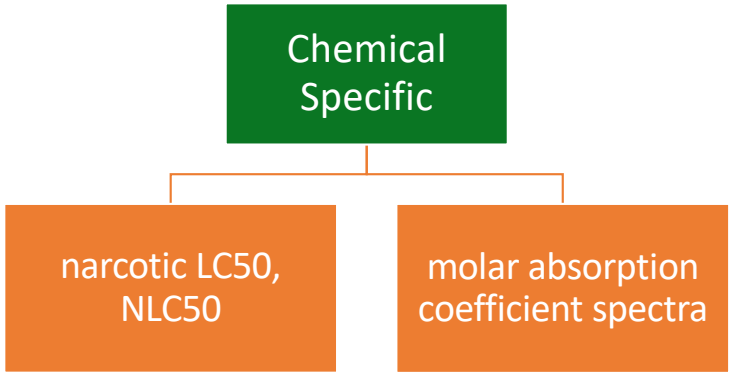
Model Structure

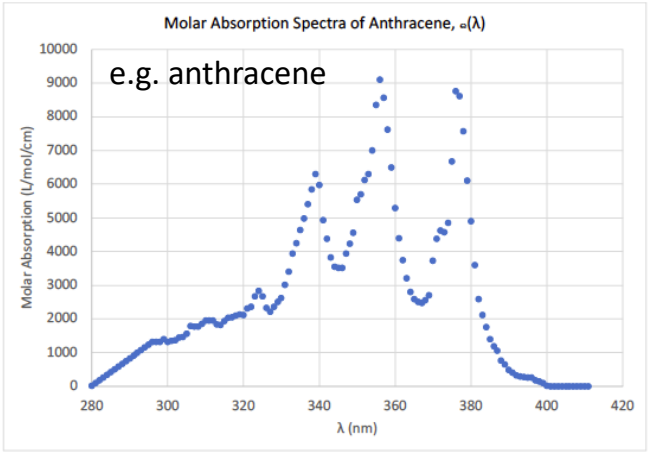


e.g. freshwater k_d model

- User input of DOC concentration (g C m^{-3})
- $k_{d,305}$ = function of [DOC]
- $S_k = 0.018\ nm^{-1}$
- $\lambda_0 = 305\ nm$

Model Structure





- 48-hour exposure, June 21 (maximum daylight)
- Model discretization
  - Time (hourly)
  - Wavelength (1 nm)
- Key assumptions and limitations

ARIS

Thank You

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