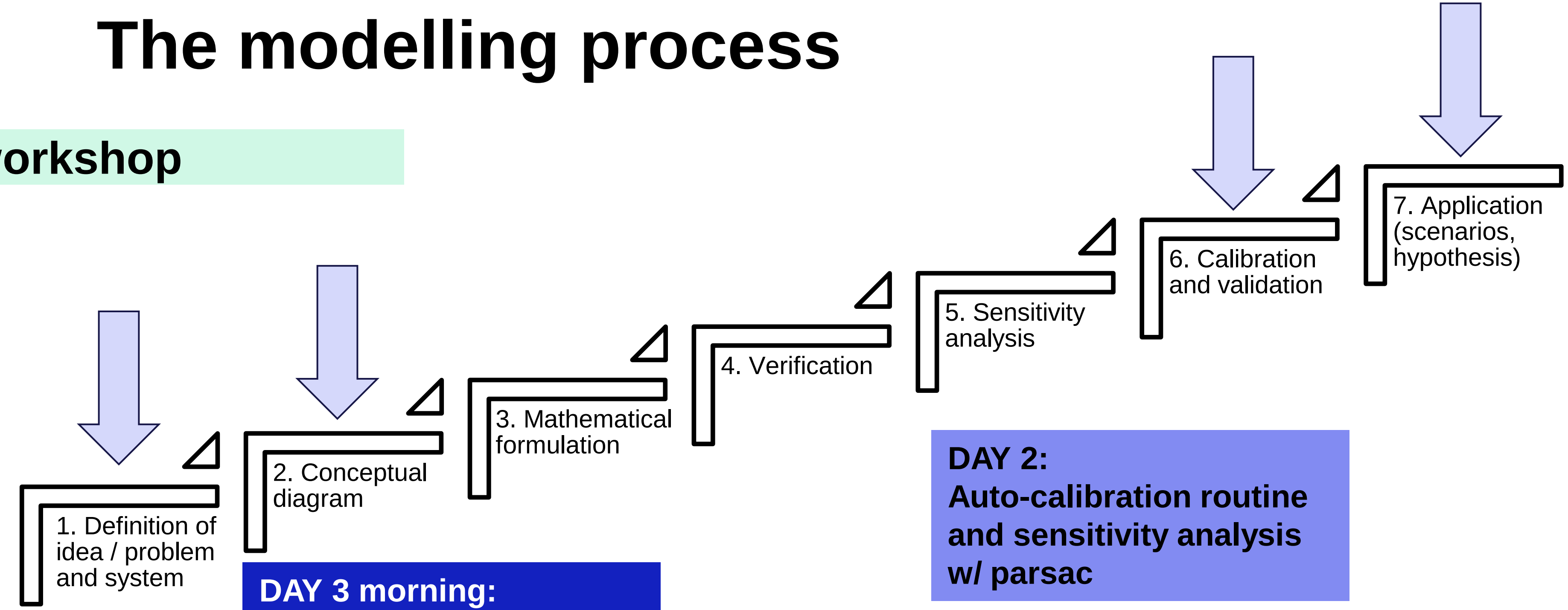
Day 2	
9:00-9:15	**Catch-up on the previous day**
9:15-10:15	**Lecture 3:** Calibrating lake ecosystems: Recommendations for WET users
10:15-10:30	Break
10:30-11:00	**Tutorial 1:** Introduction to parsac and auto-calibration
11:00-12:00	**Hands-on exercise 2:** Auto-calibration of your WET model
12:00-13:30	Break
13:30-14:00	Continue and finish exercise 2
14:00-14:45	**Tutorial 2:** Introduction to parsac and sensitivity analysis (SA)
14:45-15:00	Break
15:00-16:00	**Hands-on exercise:** Perform a SA of your WET model
16:00-16:45	**Lecture 4:** Why all modelers should do sensitivity analysis
16:45-17:00	Break
17:00-17:30	Continue and finish exercise 3
17:30-19:00	Break
19:00-21:00	**Free work session**

The modelling process

This workshop



DAY 3 morning:

WET modules and new developments to come

Code compilation and documentation

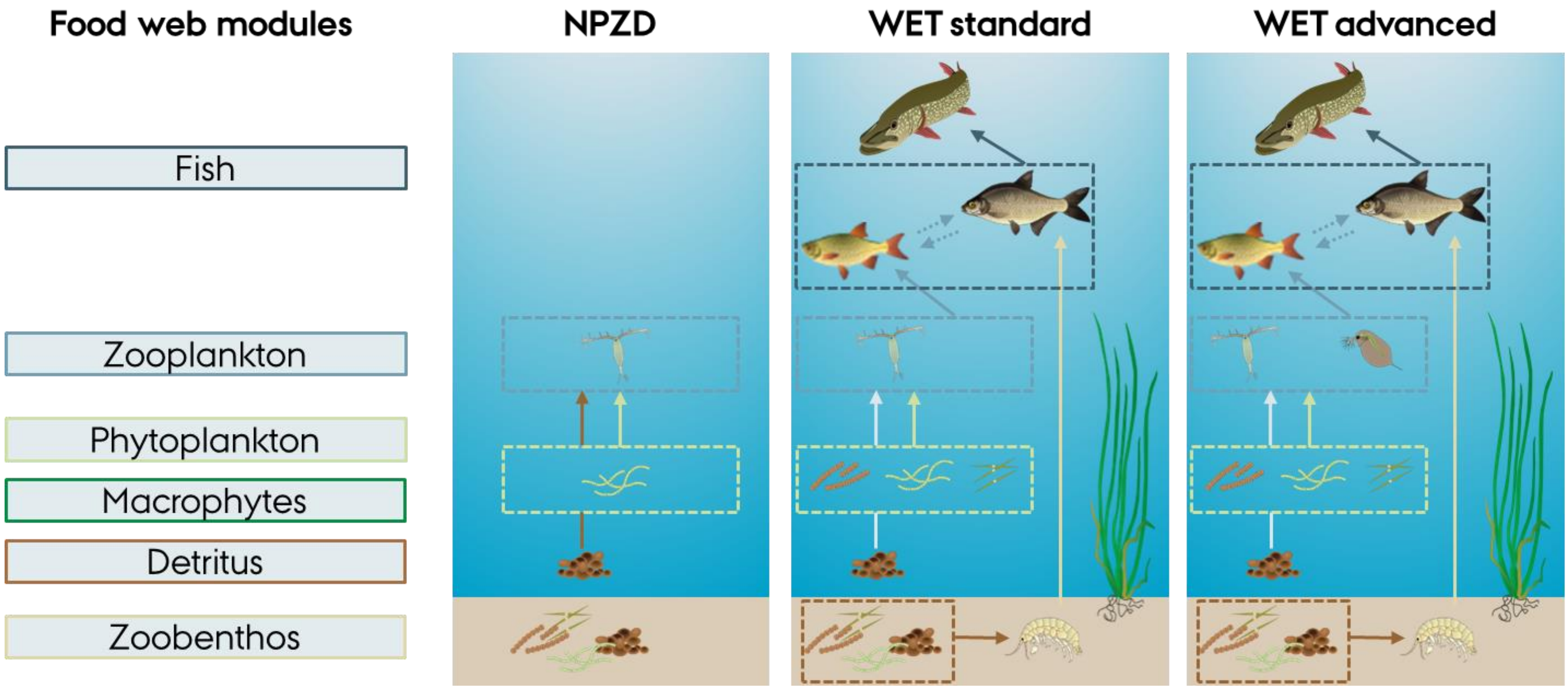
DAY 2:
Auto-calibration routine and sensitivity analysis w/ parsac

DAY 1: QWET exercise – from scratch to model set-up, simulation and scenarios

Workflow in QWET

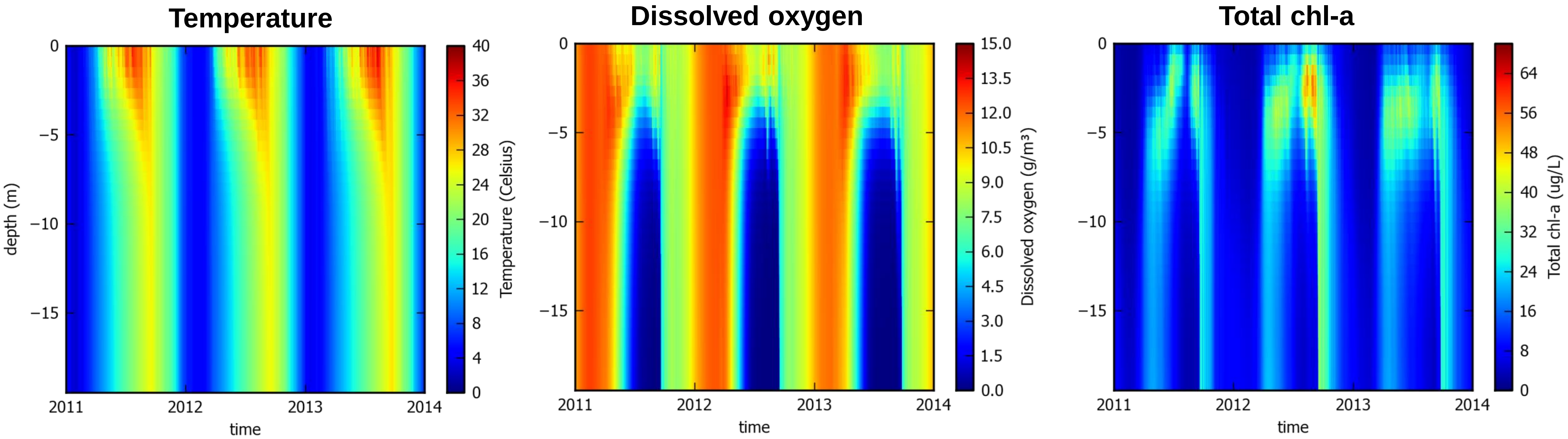
1. Model configuration and setup
2. Parameter adjustments
3. Model simulation
4. Model output visualization
   - including comparison with observations
5. Scenario design
6. Scenario simulation
7. Scenario output visualization and evaluation

RECAP: WET exercise



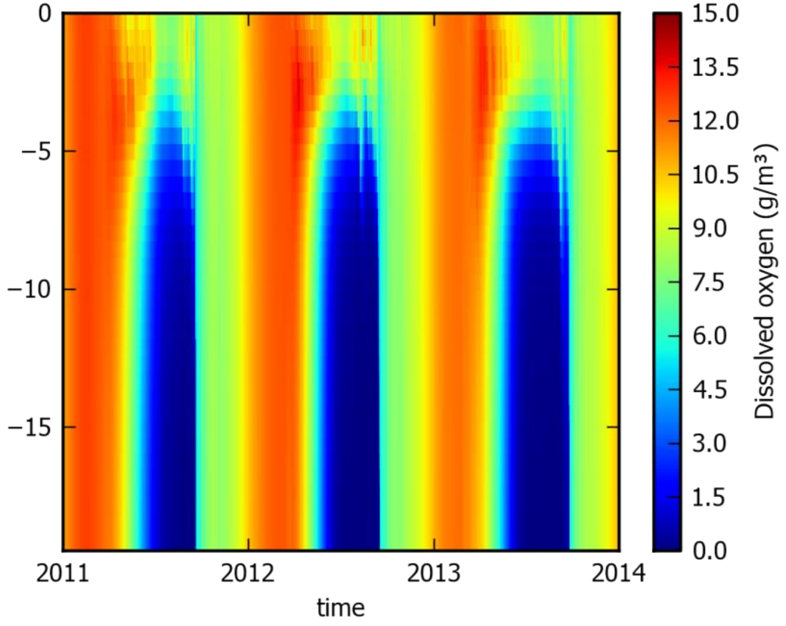
Exercise 1 results

RECAP: WET exercise

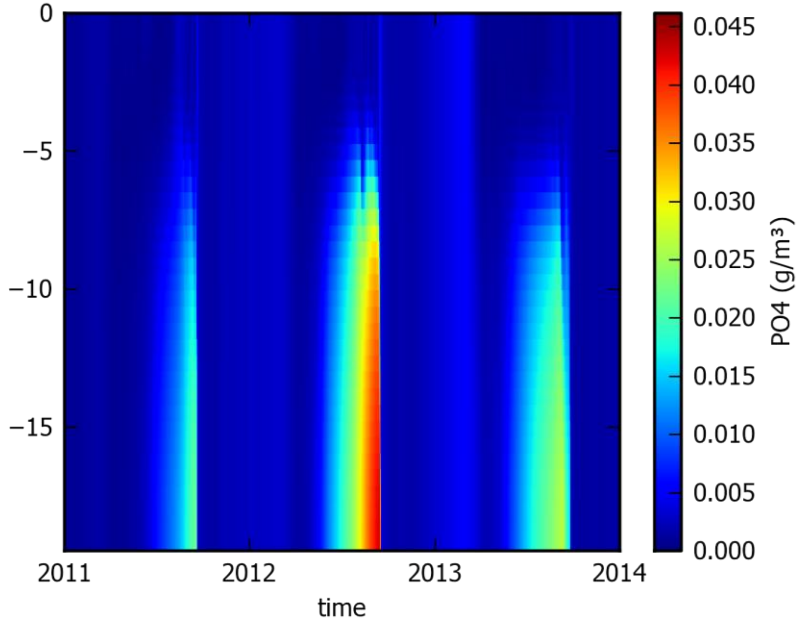


RECAP: WET exercise

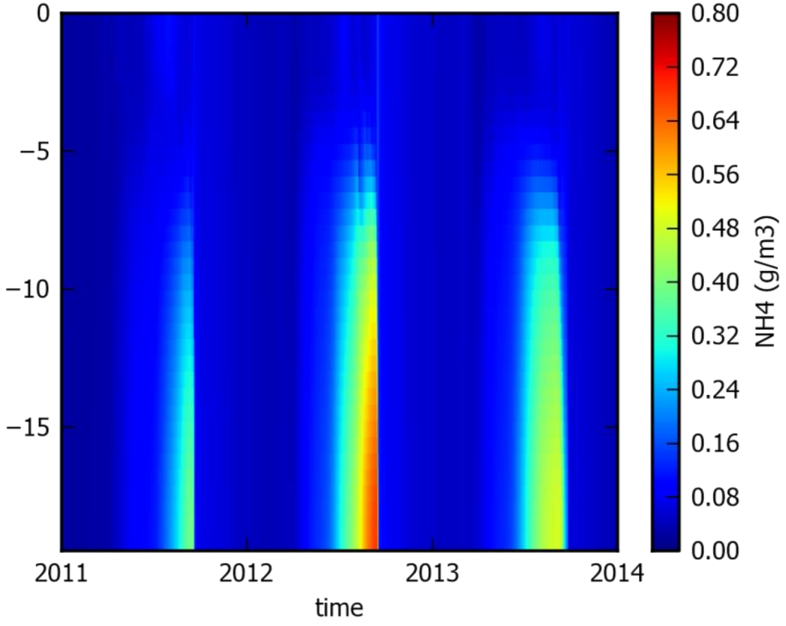
Dissolved oxygen



Phosphate (PO_4)

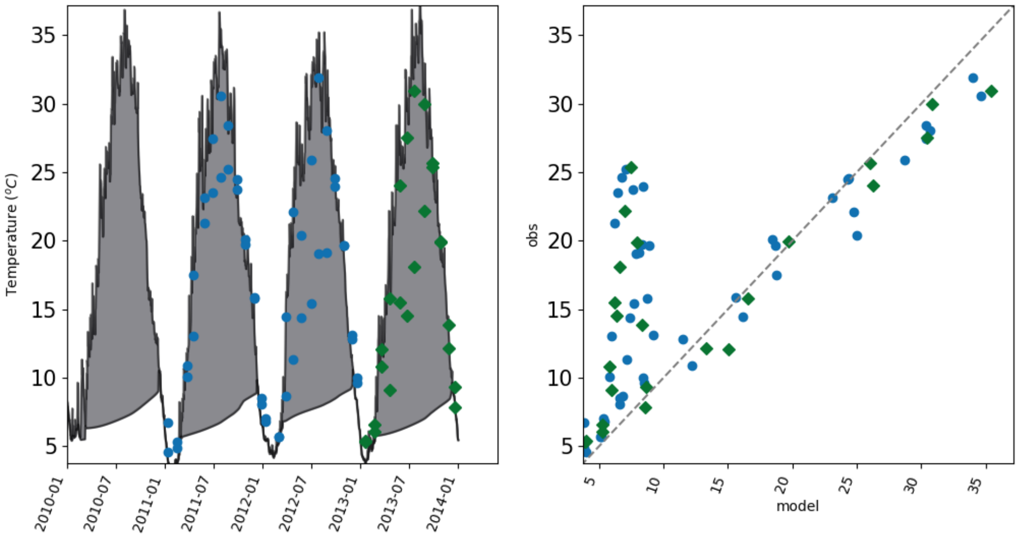


Ammonium (NH_4)

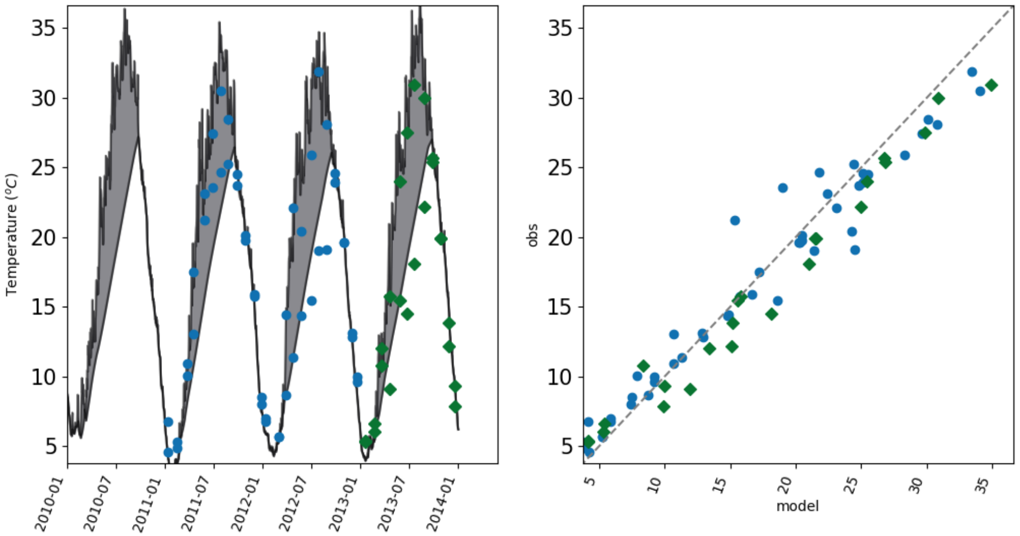


Water temperature calibration

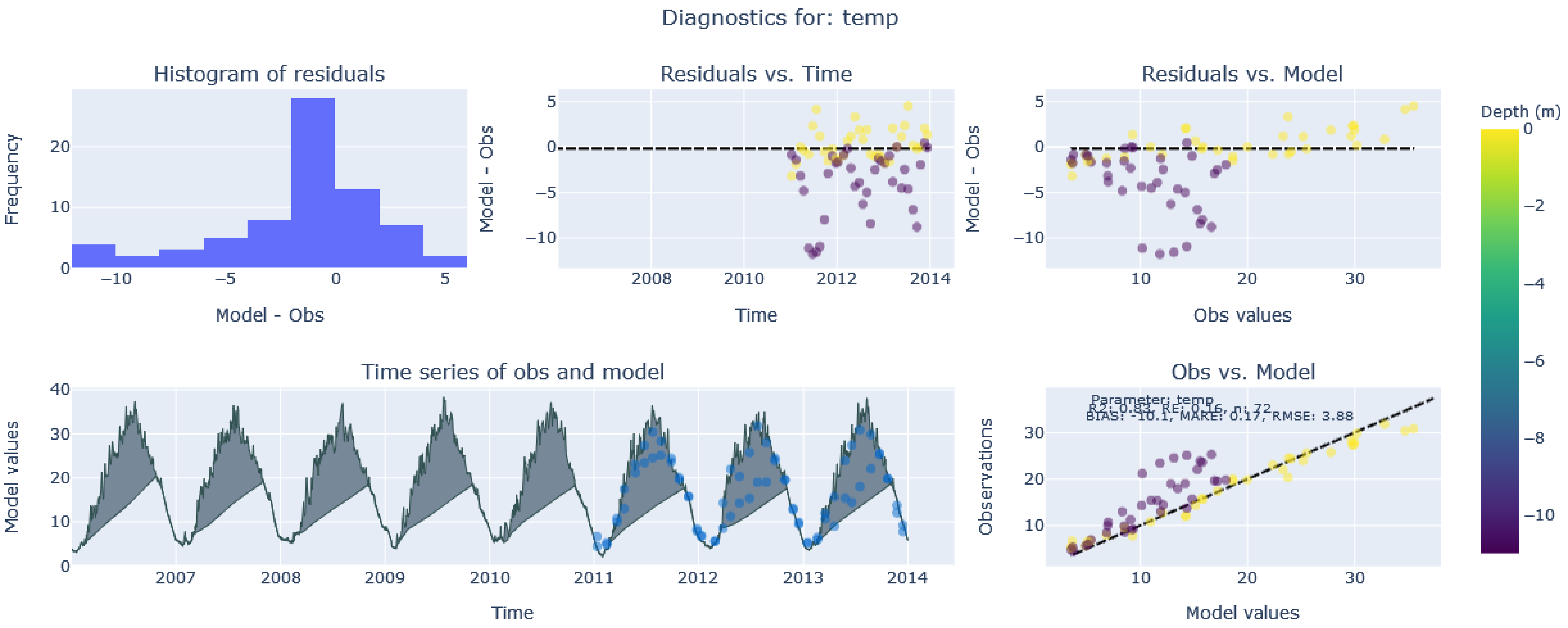
Default set-up



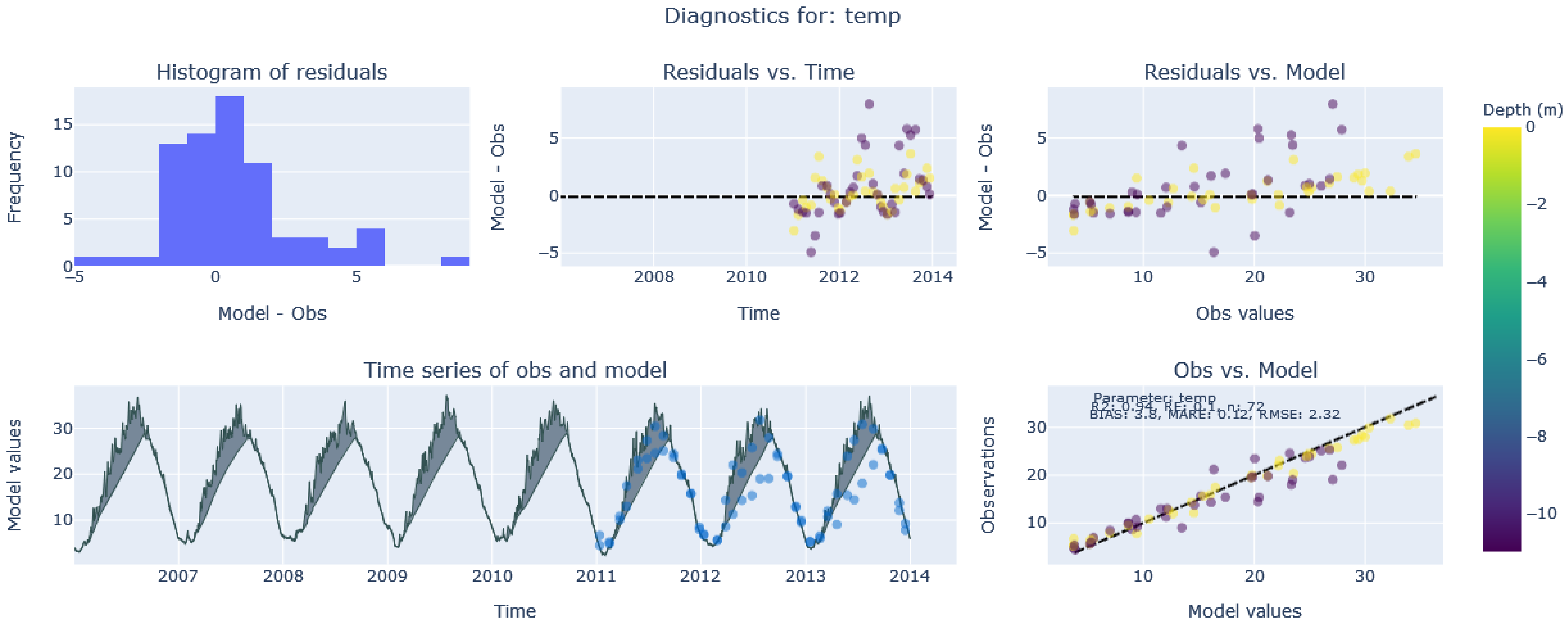
After k_min calibration



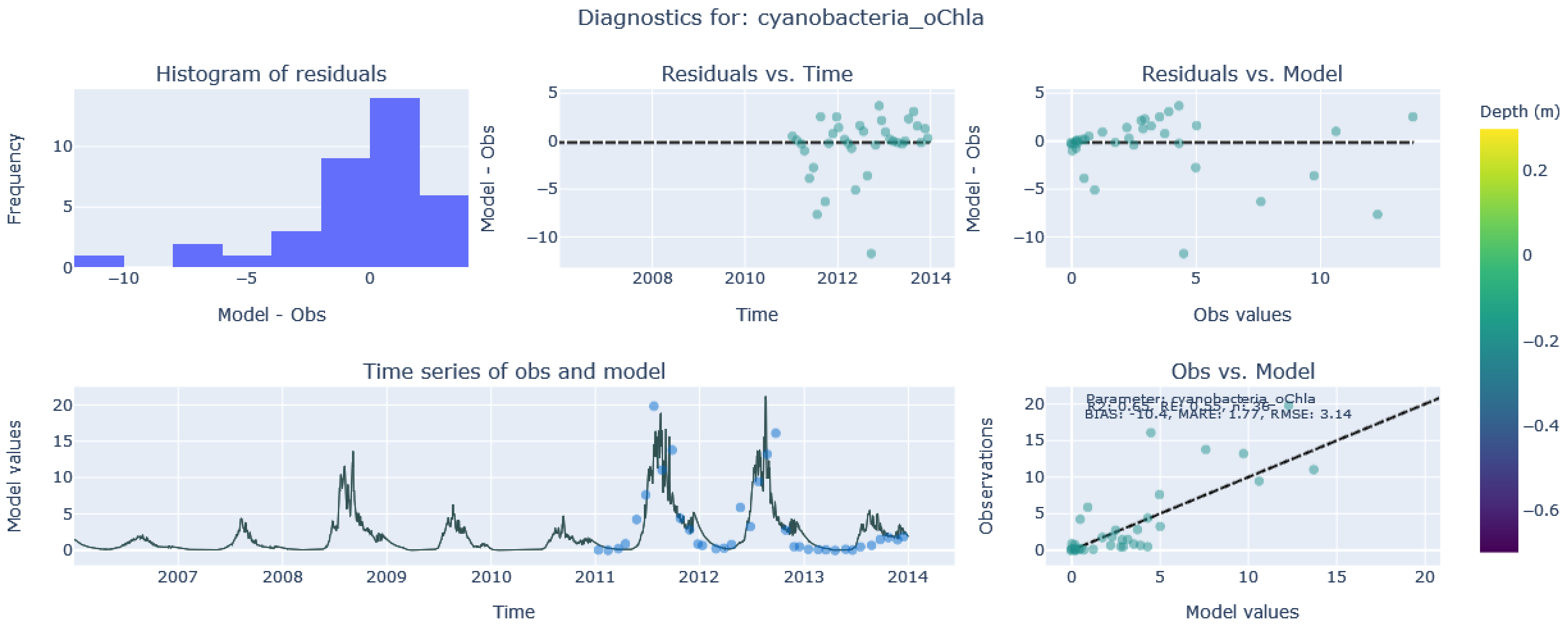
In-depth model performance diagnostics
Temperature (uncalibrated)



In-depth model performance diagnostics Temperature (calibrated)

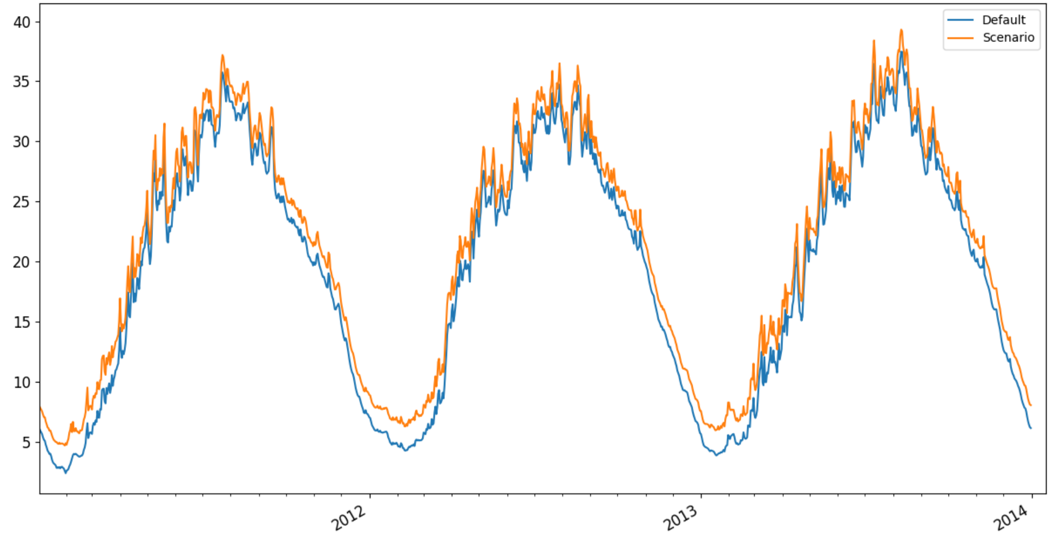


Cyanobacteria chl-a (calibrated)

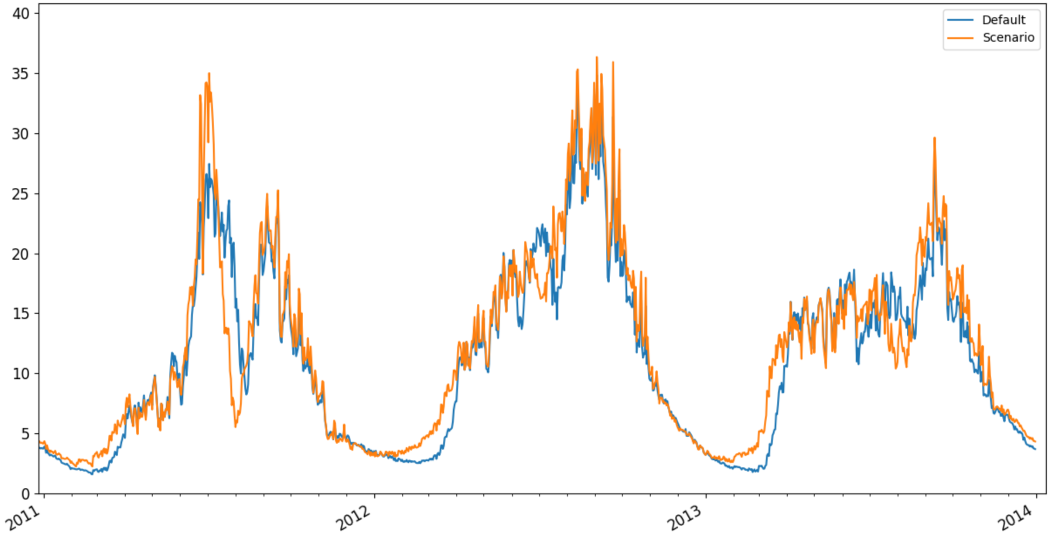


Climate warming scenario

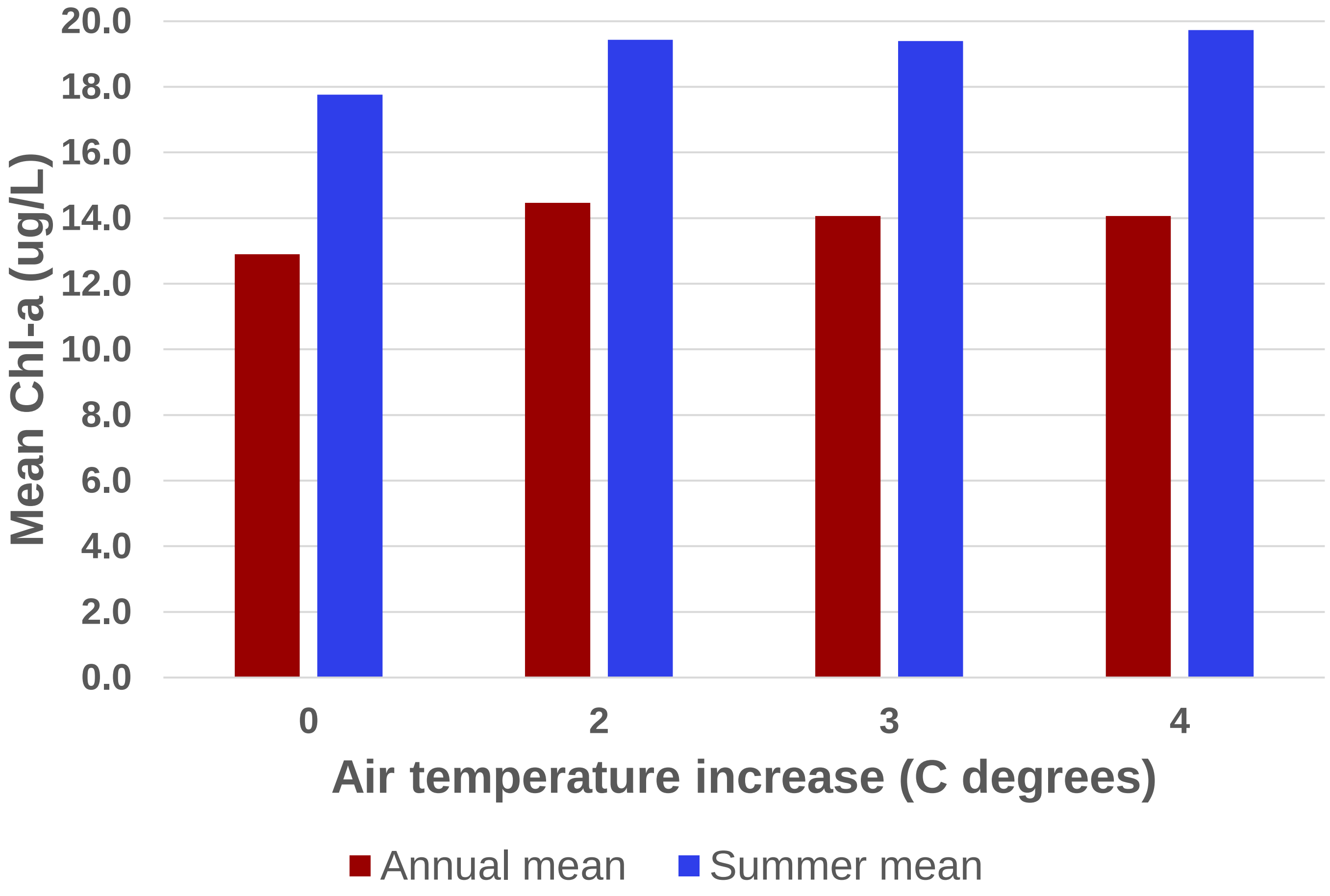
Temperature



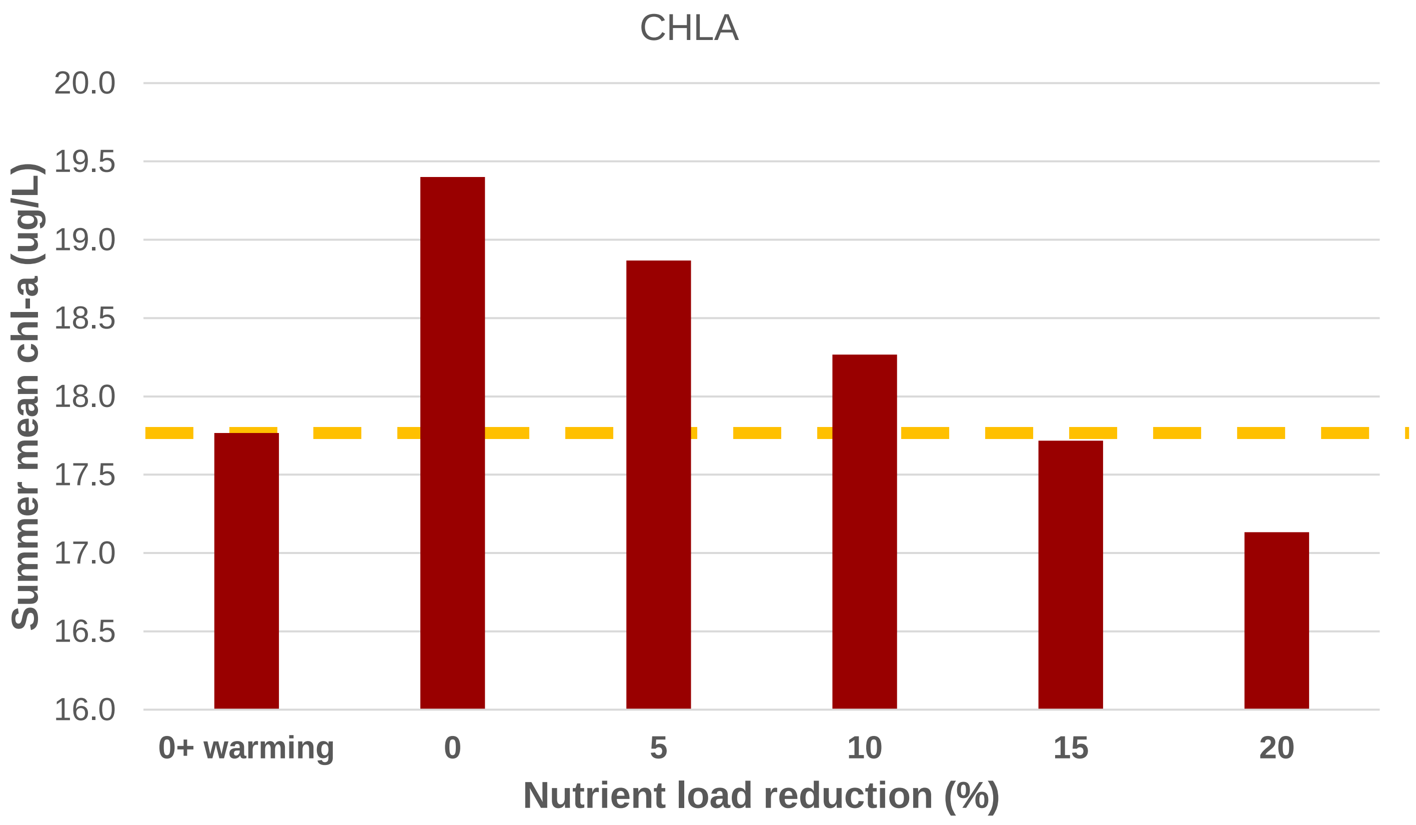
Total chl-a (ug/L)



Total chl-a response to warming



How much should we reduce external nutrient load to counteract climate warming of 3 ^{o}C?



Tobias K Andersen, Xiangzhen Kong

Calibrating lake ecosystems: Recommendations for WET users

Aim of presentation

Learning outcomes:

Participants will get an overview of

- Calibration and validation process
- Metrics and plots for model performance
- Framework for lake model evaluation
- Strategies for the calibration process
- Specific WET model considerations
- How to use SA results for the calibration

Part I

Calibration and validation – how to?

The modelling process

1. Definition of idea / problem and system
2. Conceptual diagram
3. Mathematical formulation
4. Verification
5. Sensitivity analysis
6. Calibration and validation
7. Application (scenarios, hypothesis)

Why is model validation important?

- Falsifiability is a fundamental principle in science:
  - Karl Popper: *scientific theories and hypotheses must be capable of being proven false in order to be considered valid (falsifiability)*
  - A model must be subjected to rigorous testing
  - If a model cannot be falsified, then it cannot be considered a valid scientific or mathematical model.
- Epistemological humility
  - recognize that there are limits to what we can know and predict
- Ethics and accountability
  - If used for decision-making then it is crucial that they are validated and tested rigorously to ensure that they are not biased (or discriminatory)

Why is model validation important?

- Models must be validated for several reasons
  - Increase scientific credibility
  - Detect errors
  - Assess accuracy
  - Determine the validity range of the model

- All scientific models are capable of being validated (falsified)
- But the specific validation practices depends on model type and purpose of the model

Calibration and validation

6. Calibration and validation

"**Calibration** is adjusting model parameters with the purpose of achieving the best simulation match with observations."

This may be achieved by a combination of visual inspection and optimization of an objective function.

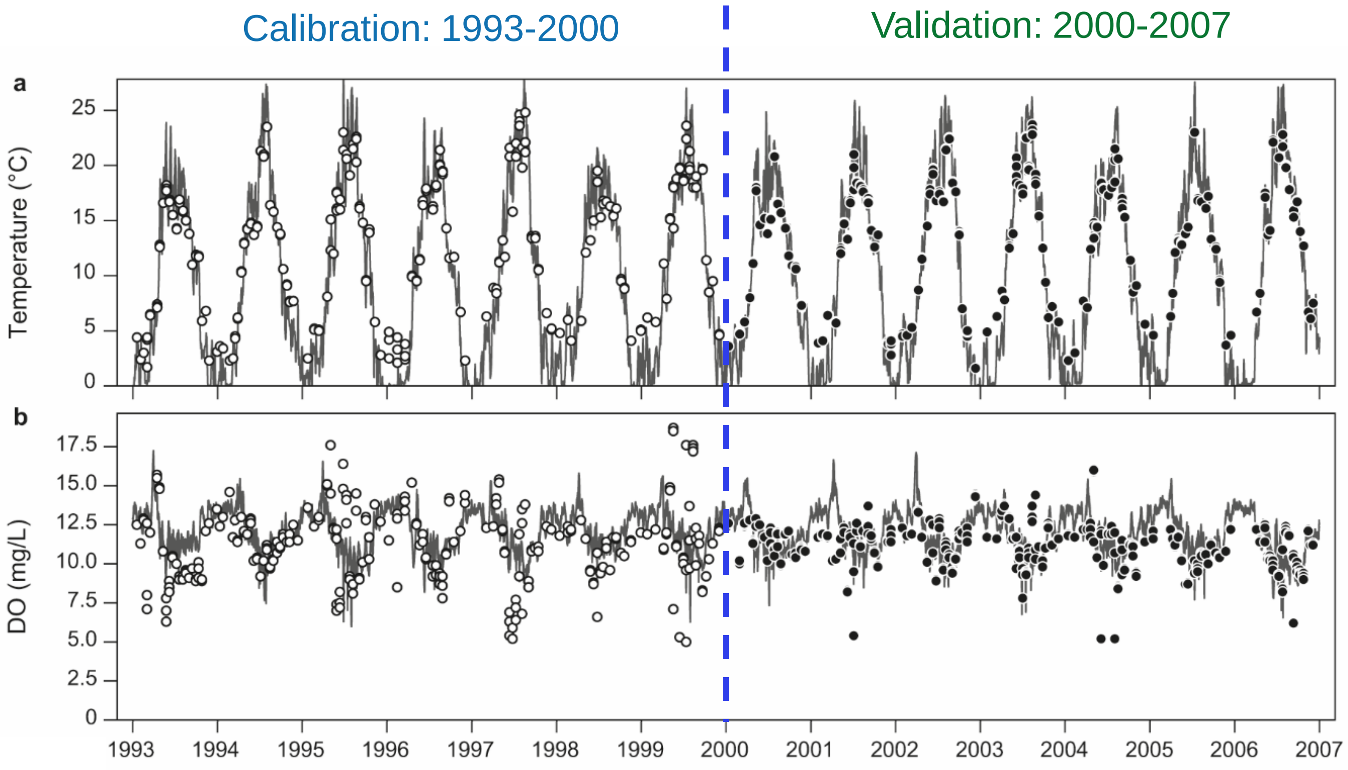
For example, minimizing the
Mean Absolute Percentage Error (MAPE):

$$MAPE(Chla) = \frac{1}{n}\sum_{i=1}^{n}\frac{\left|Chla_{simulated} - Chla_{observed}\right|}{Chla_{observed}}$$

6. Calibration and validation

"**Validation** is the process of testing the calibrated parameters with an independent set of data (in time and/or space)"

Model adjustment to Lake Hinge case

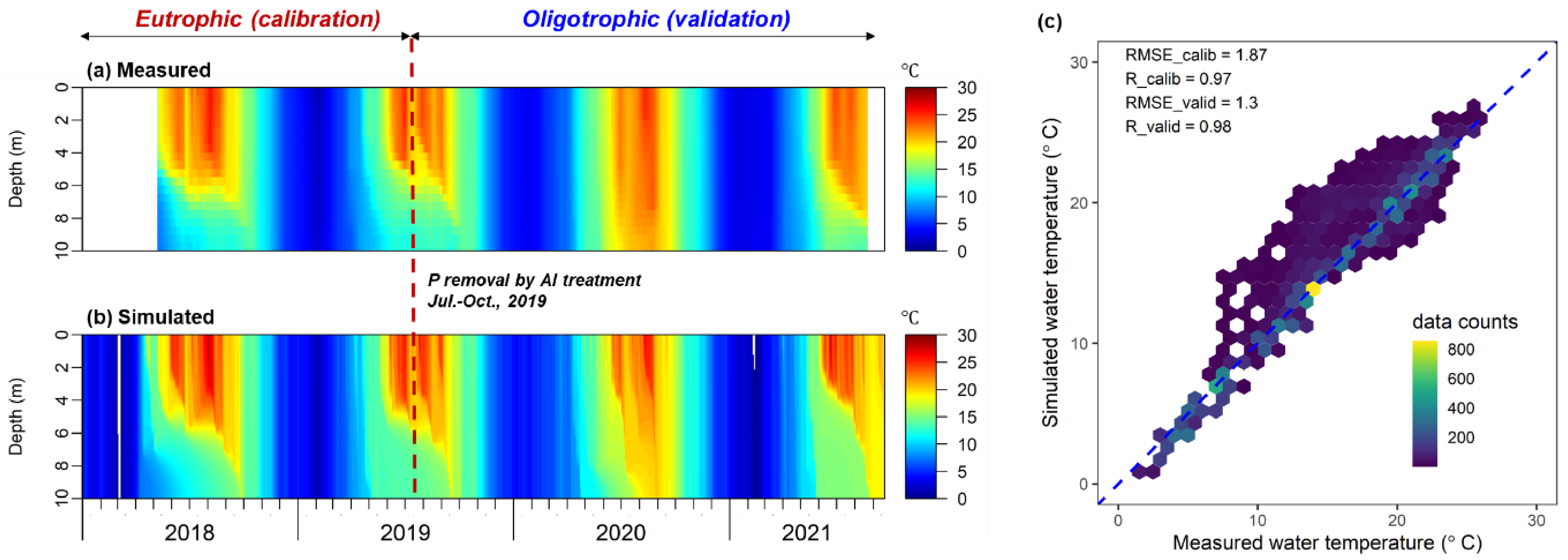


Andersen et al, 2020, *Ecol. Appl.*

Calibration and validation

6. Calibration and validation

Model adjustment to Lake Barleber case



Kong et al., ES&T 2023

Calibration and validation

6. Calibration and validation

Choosing objective functions (model performance metrics) for calibration and validation

"an **objective function** is a mathematical expression for how closely model output matches observations"

The different types of model performance metrics have both strengths and weaknesses. Multiple performance metrics should therefore always be evaluated – ideally combining residual and correlation type metrics. For example, the coefficient of determination r^2, which can suffer significant offset error, could be paired with percent bias (Bennett et al. 2013).

Calibration and validation

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Performance metrics

6. Calibration and validation

Choosing objective functions (model performance metrics) for calibration and validation

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Environmental Modelling & Software

Position paper

Characterising performance of environmental models

1. Introduction

Bennett et al (2013)
Environ. Model. Softw.

The different types of model performance metrics have both strengths and weaknesses. Multiple performance metrics should therefore always be evaluated – ideally combining residual and correlation type metrics. For example, the coefficient of determination r^2, which can suffer significant offset error, could be paired with percent bias (Bennett et al. 2013).

Examples of commonly used **residual performance metrics**:

- Used to calculate the difference between observed and modelled data points

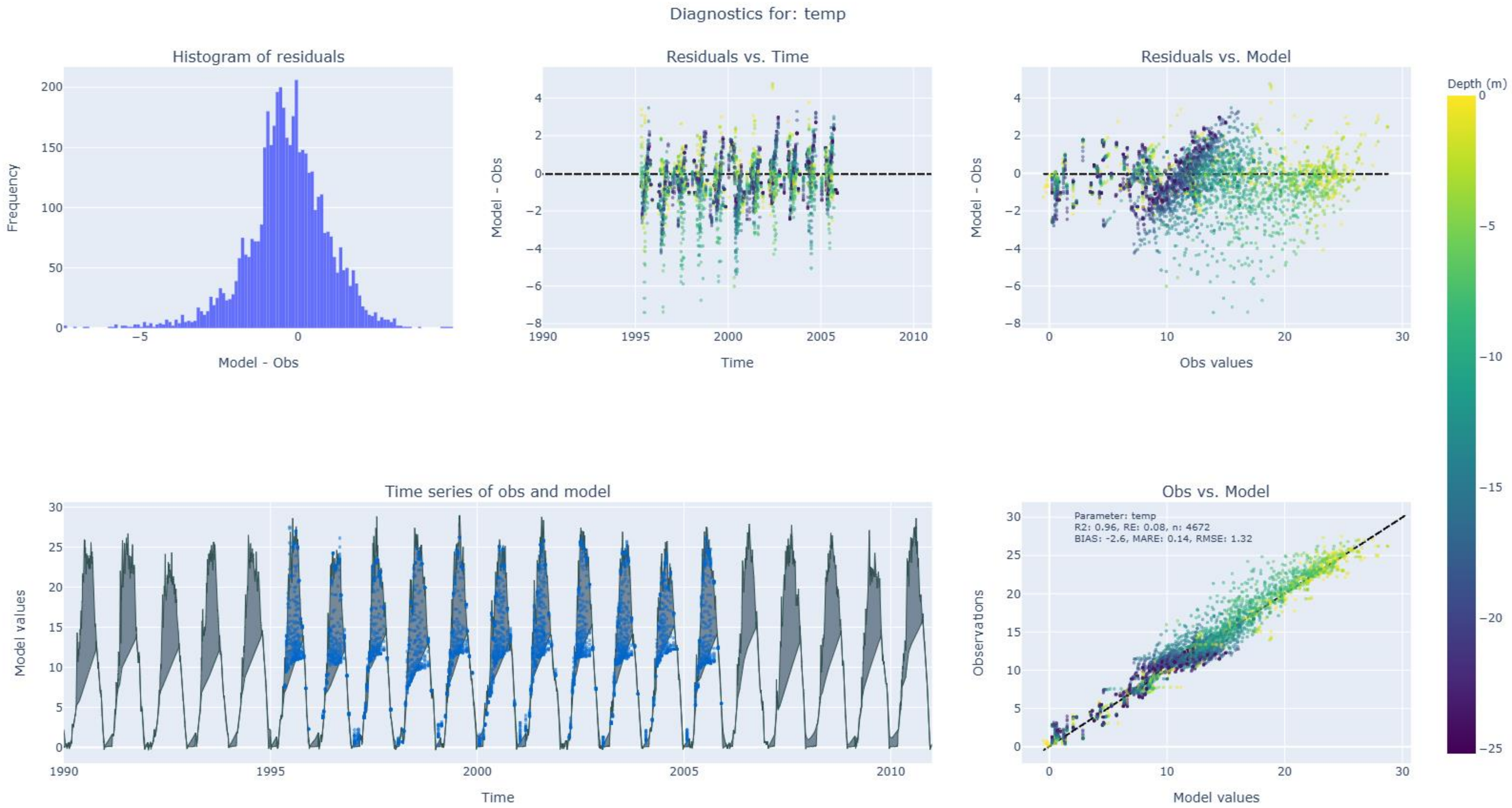
- Root Mean Square Error (RMSE)
- Mean Absolute Error (MAE)
- Bias (or percent bias)

Examples of commonly used **correlation and model efficiency performance metrics**:

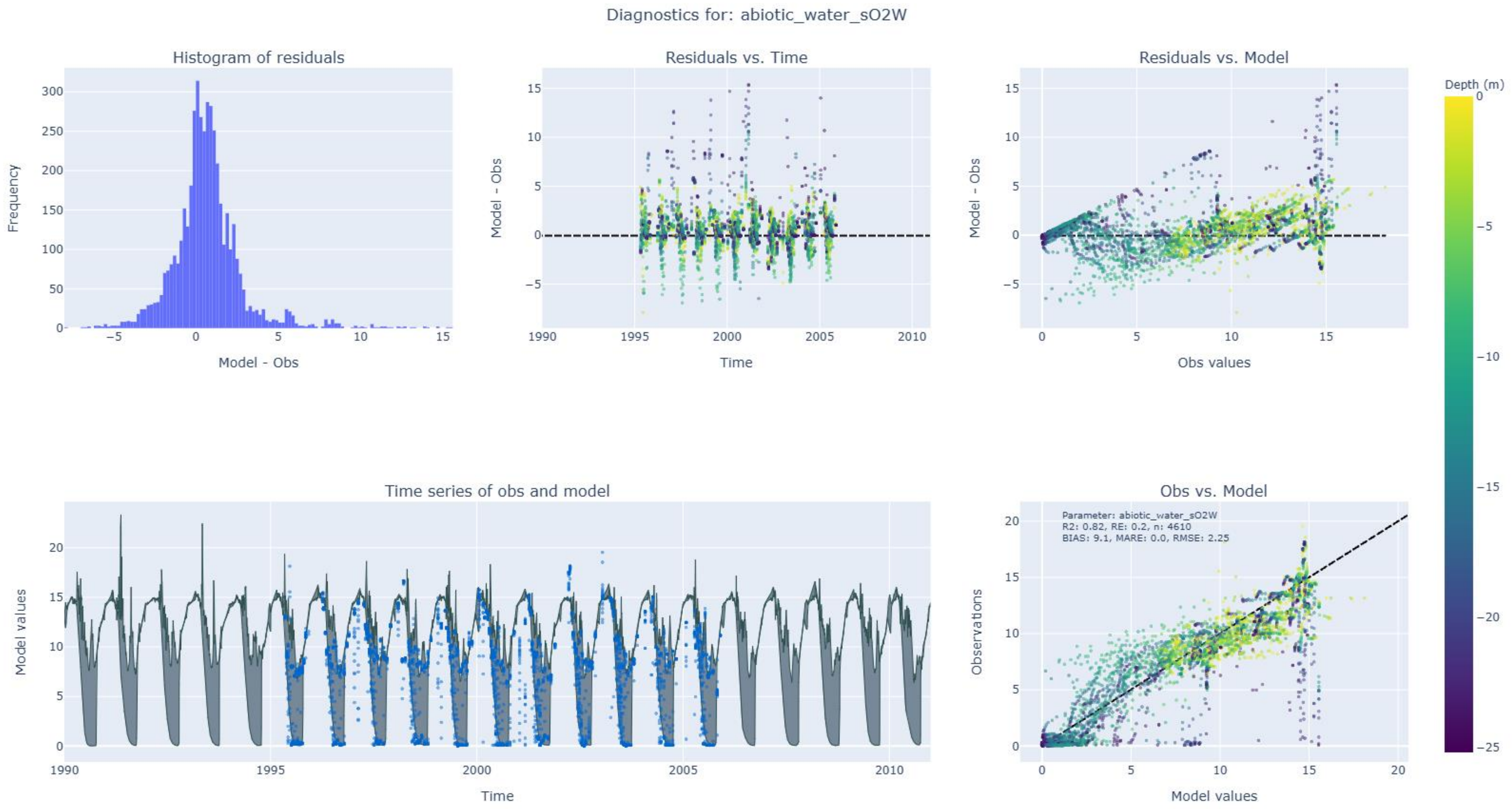
- Used to test ability to preserve patterns observed in data

- Pearson Product moment correlation (r)
- Coefficient of determination (**r^2**)
- Nash-Sutcliffe efficiency coefficient (**NSE**)

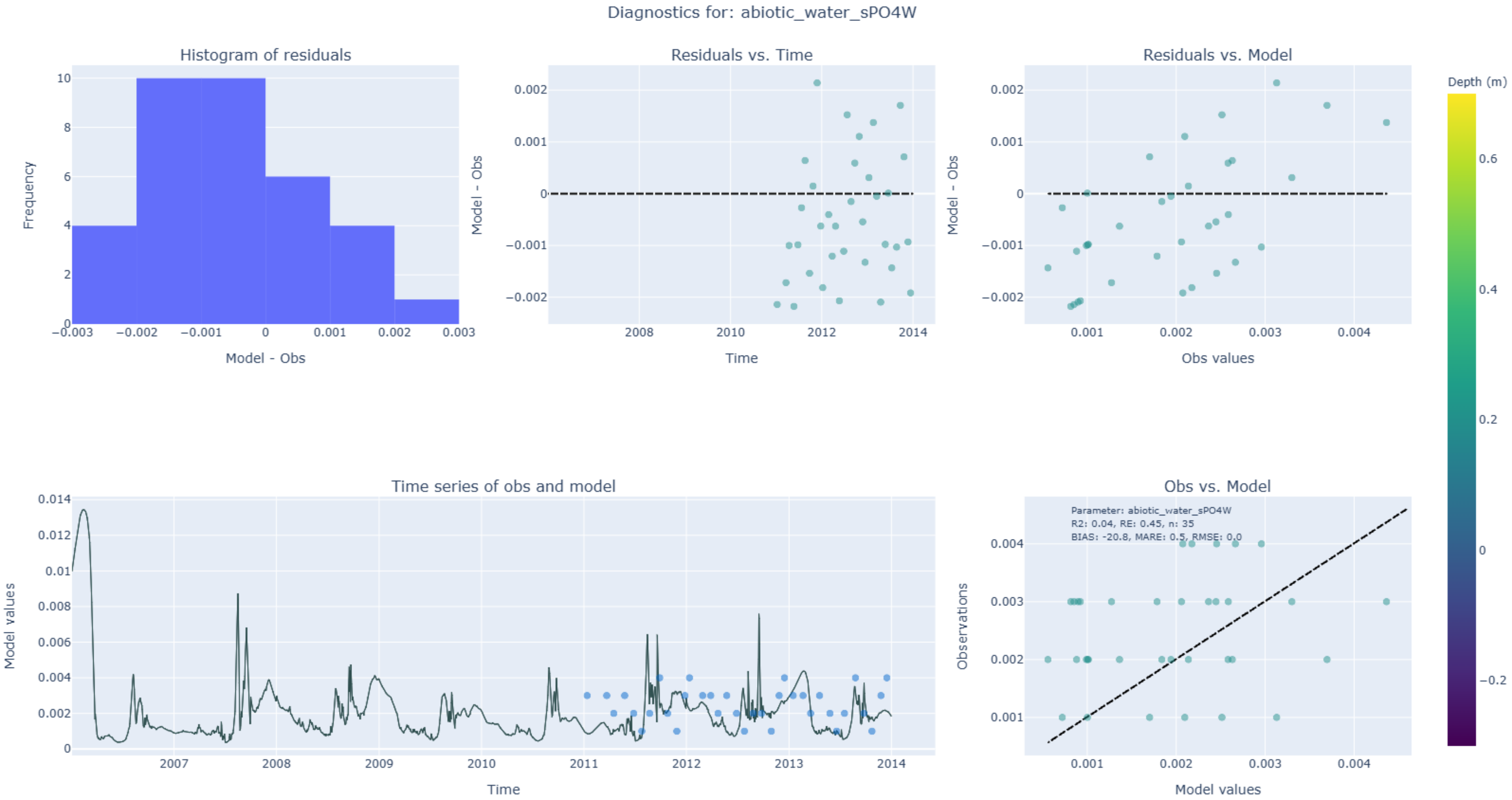
Performance visualizations



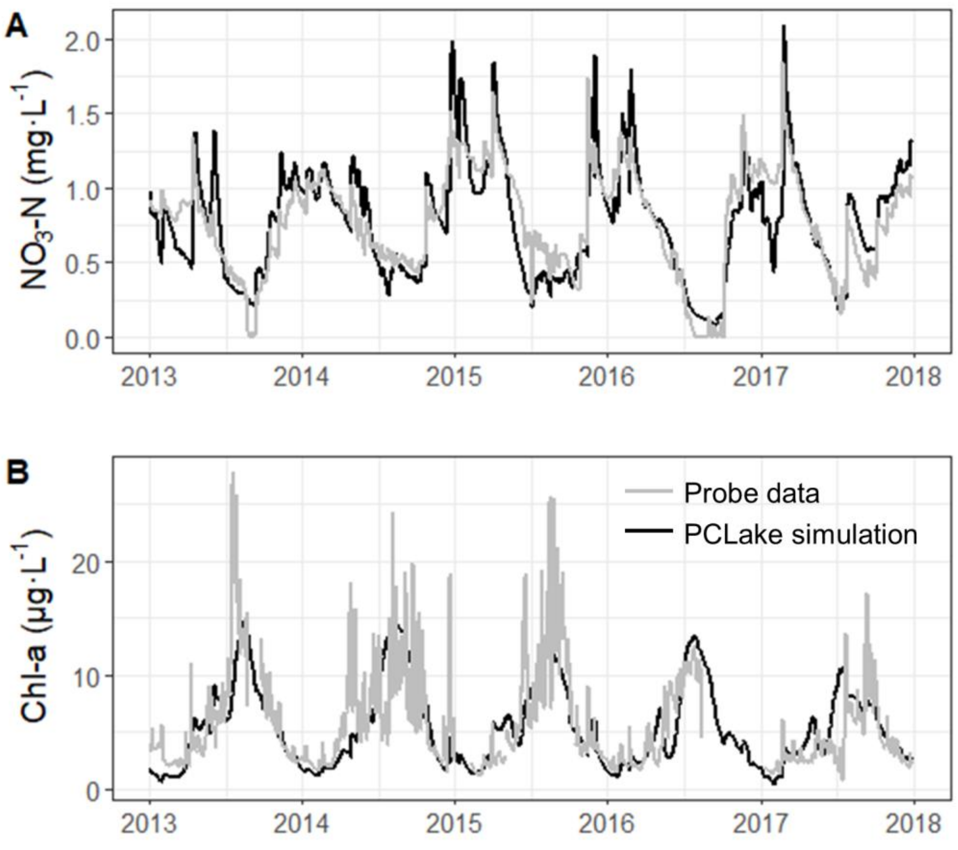
Performance visualizations



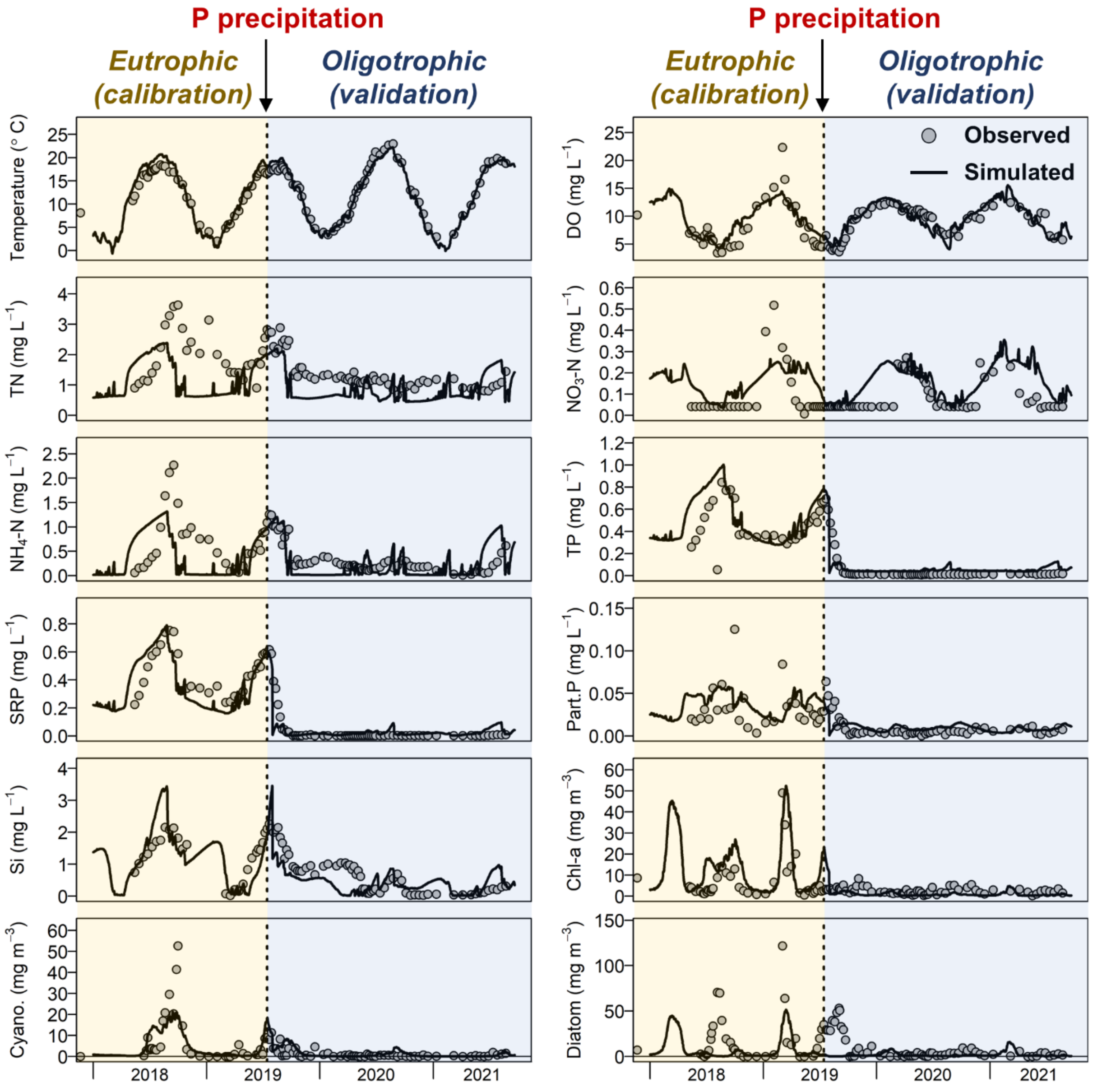
Performance visualizations



Performance visualizations



Kong et al., Water Res. 2019



Kong et al., ES&T 2023

Part II

Evaluating lake model performance: What and why?

Model evaluation: The fundamentals

Model evaluation is always tightly linked to model purpose.

> *"All models are approximations. Assumptions, whether implied or clearly stated, are never exactly true.* ***All models are wrong, but some models are useful****. So the questions you need to ask is not "Is the model true?" (it never is) but "Is the model good enough for this particular application?"*
>
> George Box

Modelers need to ask:

"What makes the model fit-for-purpose?"

Model evaluation: The fundamentals

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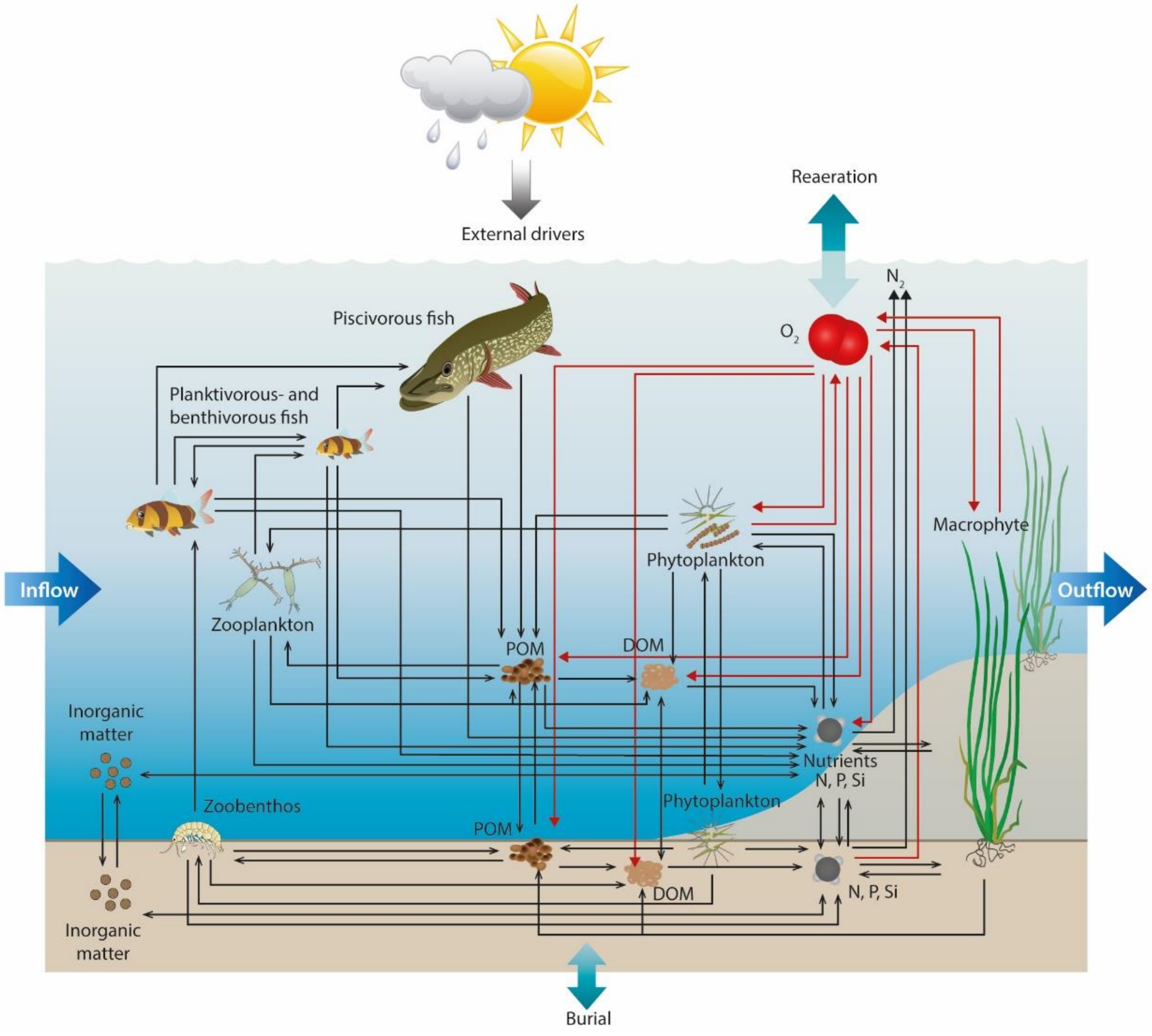
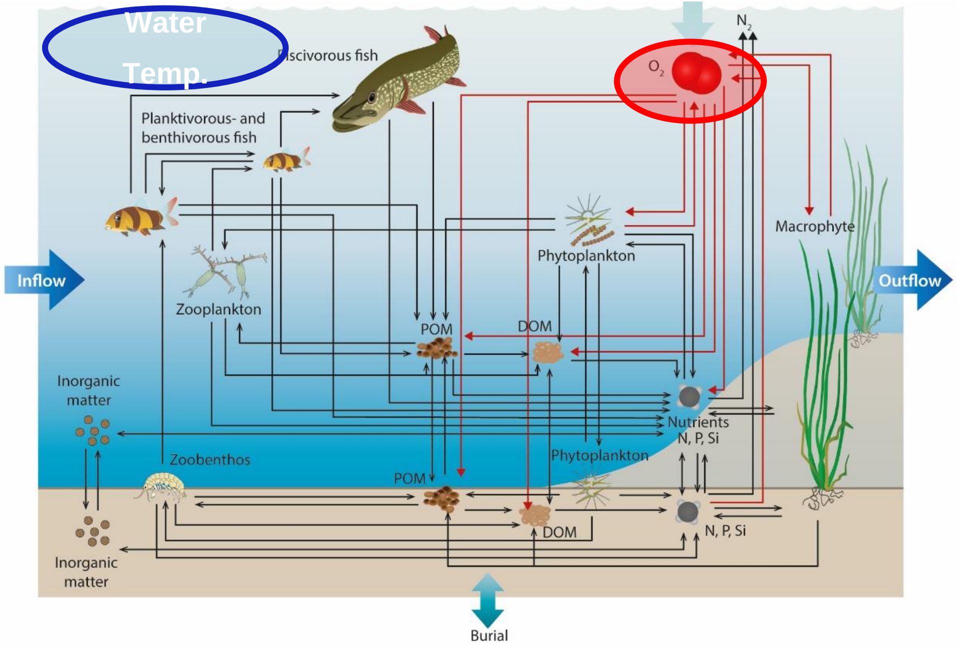
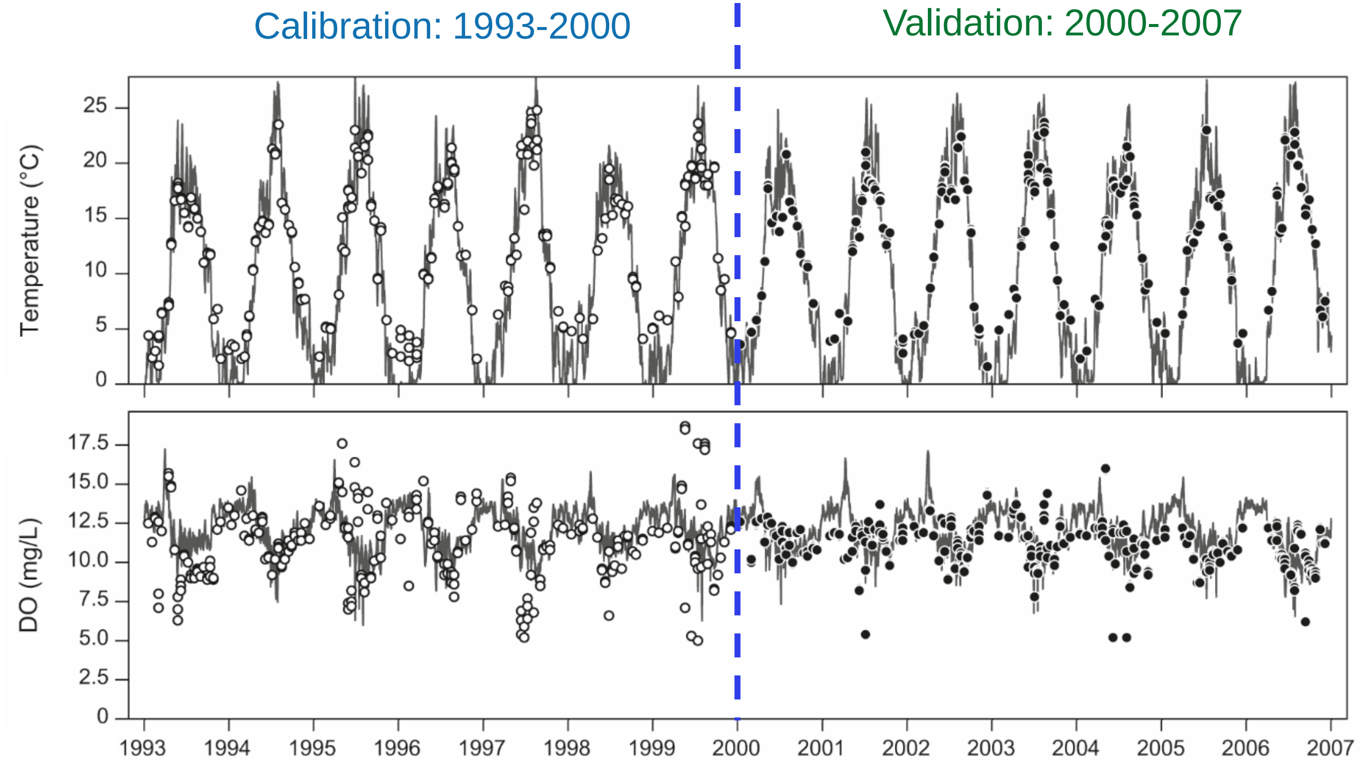


WQ state variables





Andersen et al, 2020, *Ecol. Appl.*

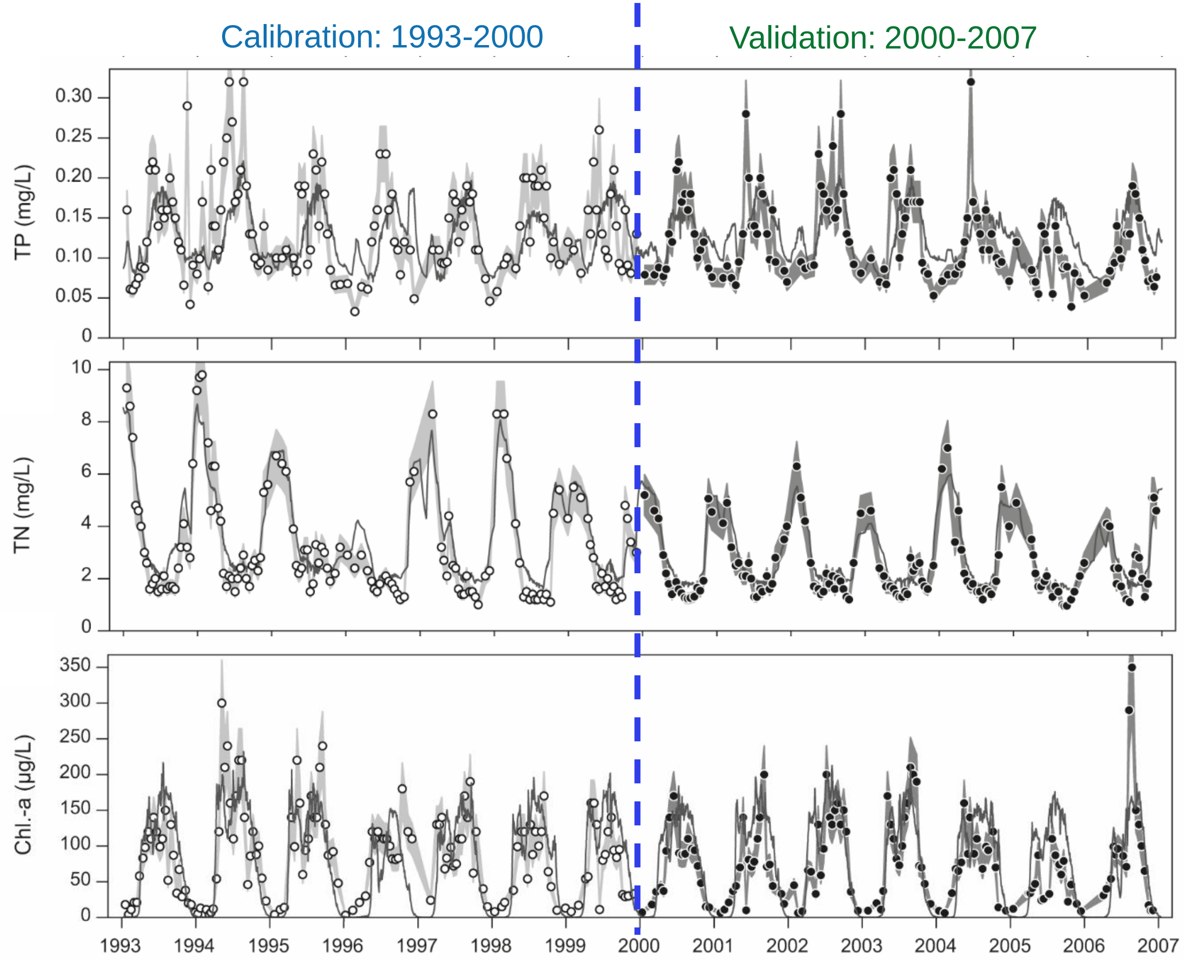
R^2: 0.96|0.98

BIAS (%): -2.0| 2.3

R^2: 0.18|0.21

BIAS (%): 6.0| 5.1

WQ state variables



Andersen et al, 2020, *Ecol. Appl.*

R^2: 0.24|0.32

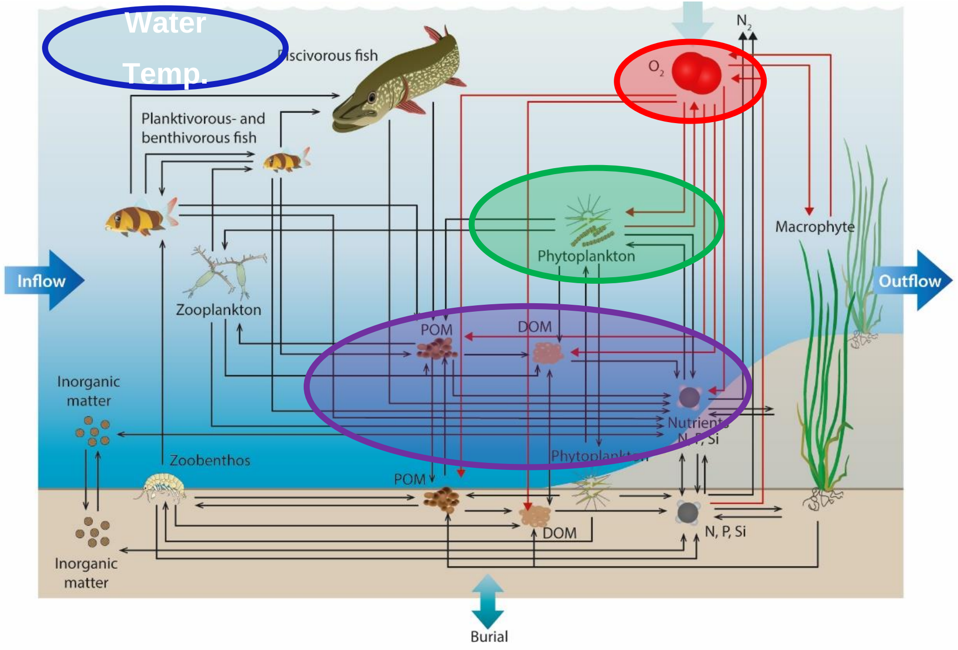
BIAS (%): -5.1| 8.0

R^2: 0.89|0.83

BIAS (%): 10.8| 9.7

R^2: 0.43|0.43

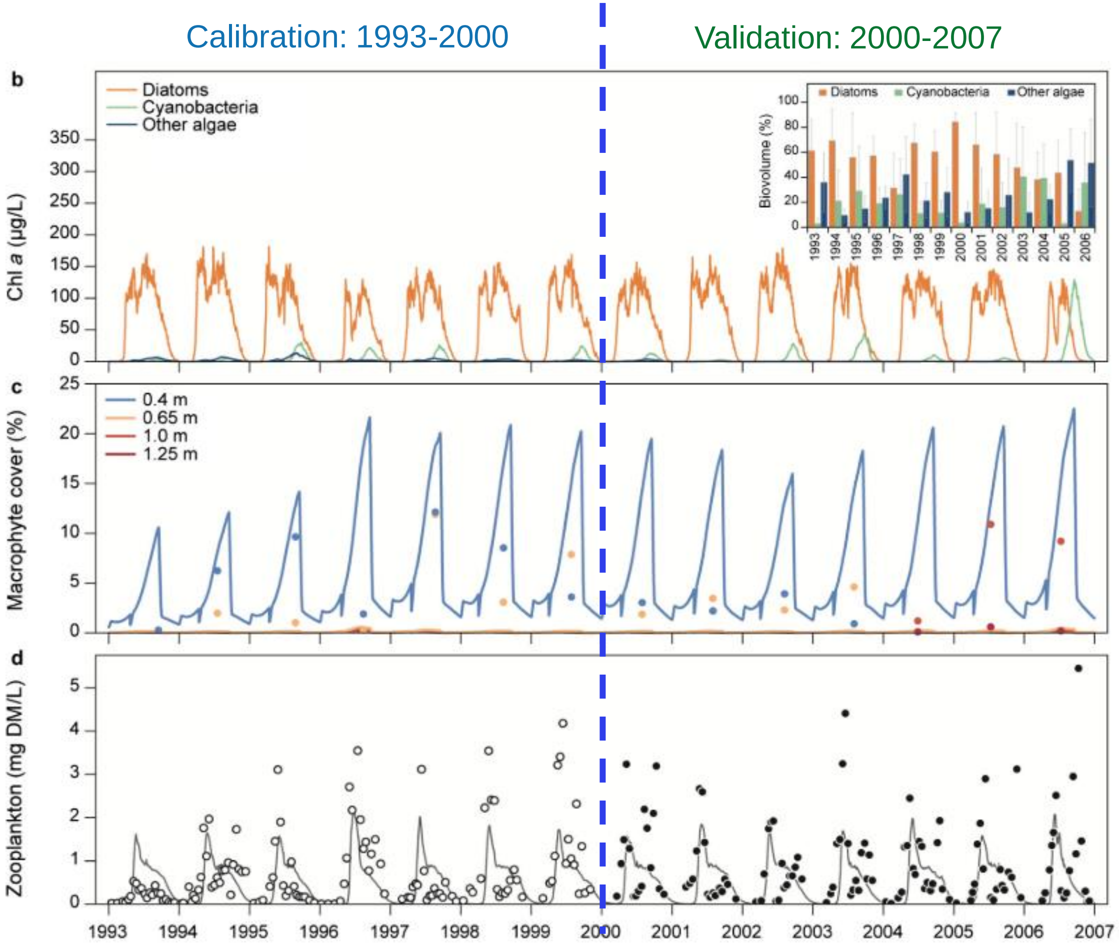
BIAS (%): -6.6| 6.0



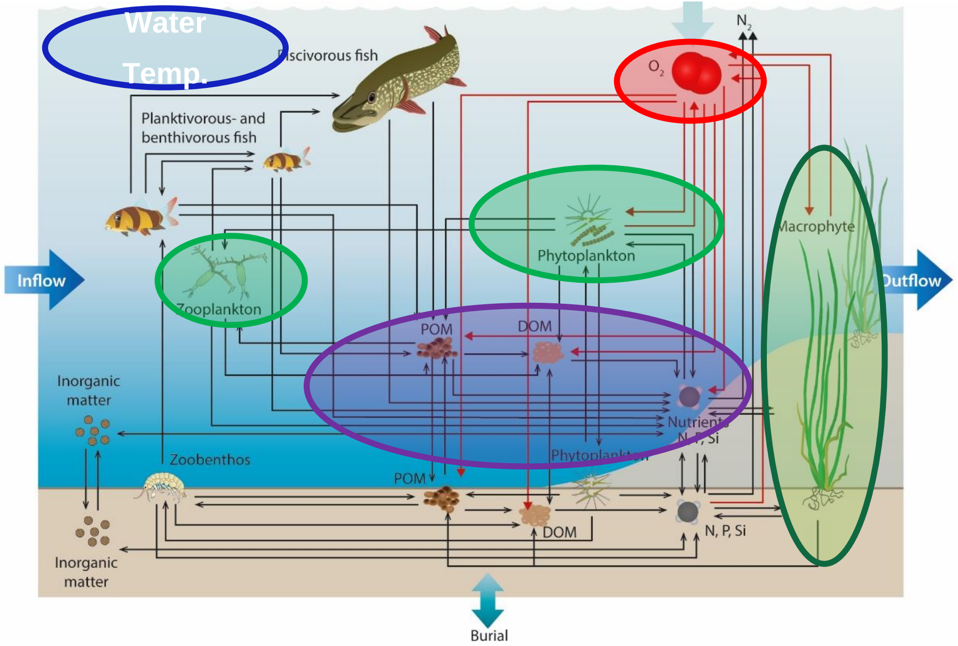
WQ state variables

Calibration: 1993-2000

Validation: 2000-2007

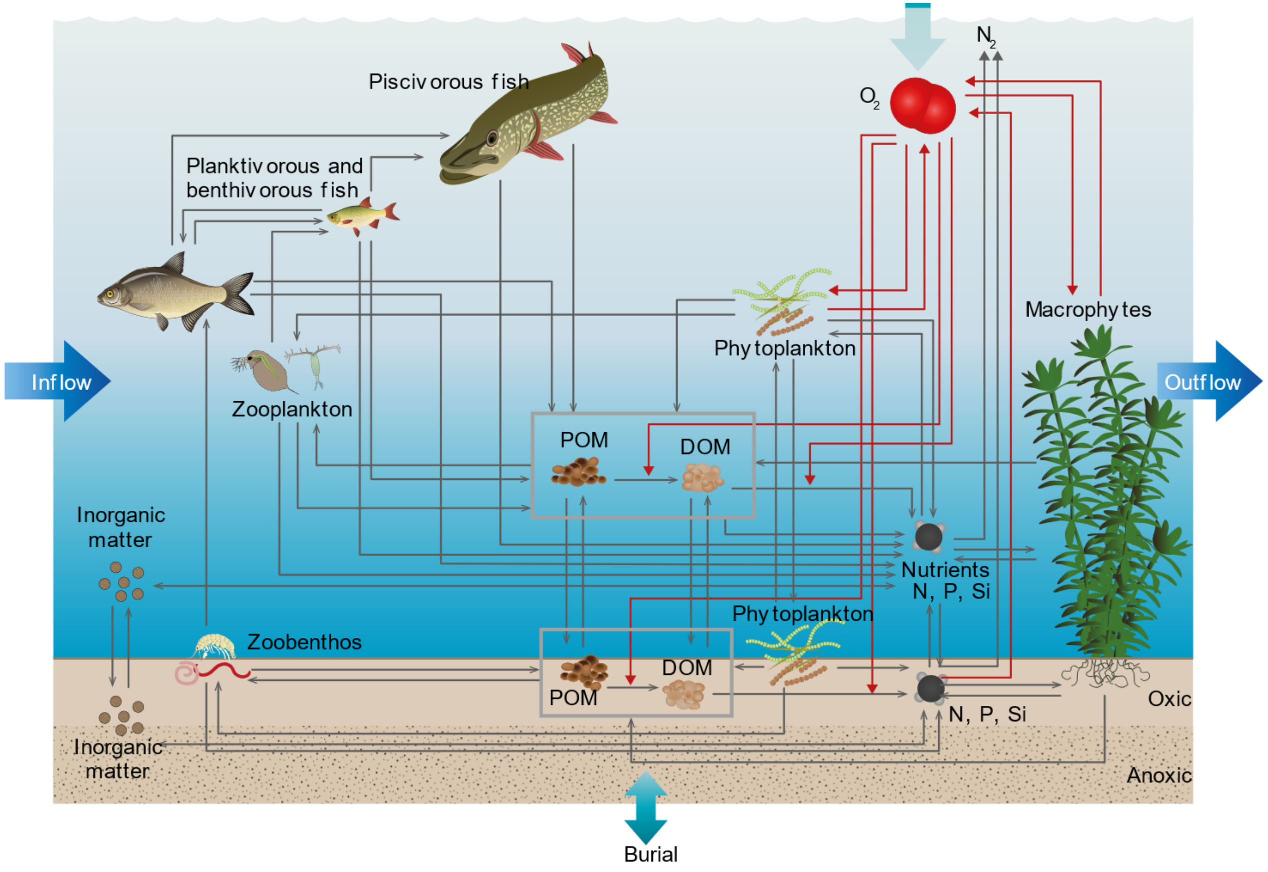


Andersen et al, 2020, *Ecol. Appl.*

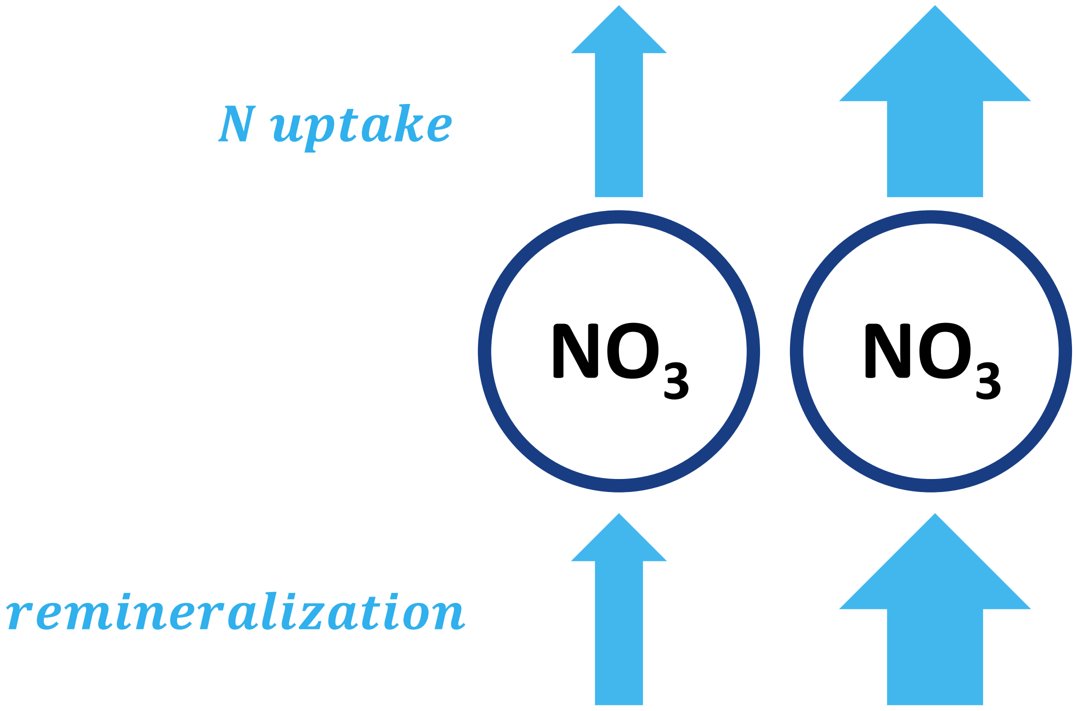


Model evaluation: The fundamentals

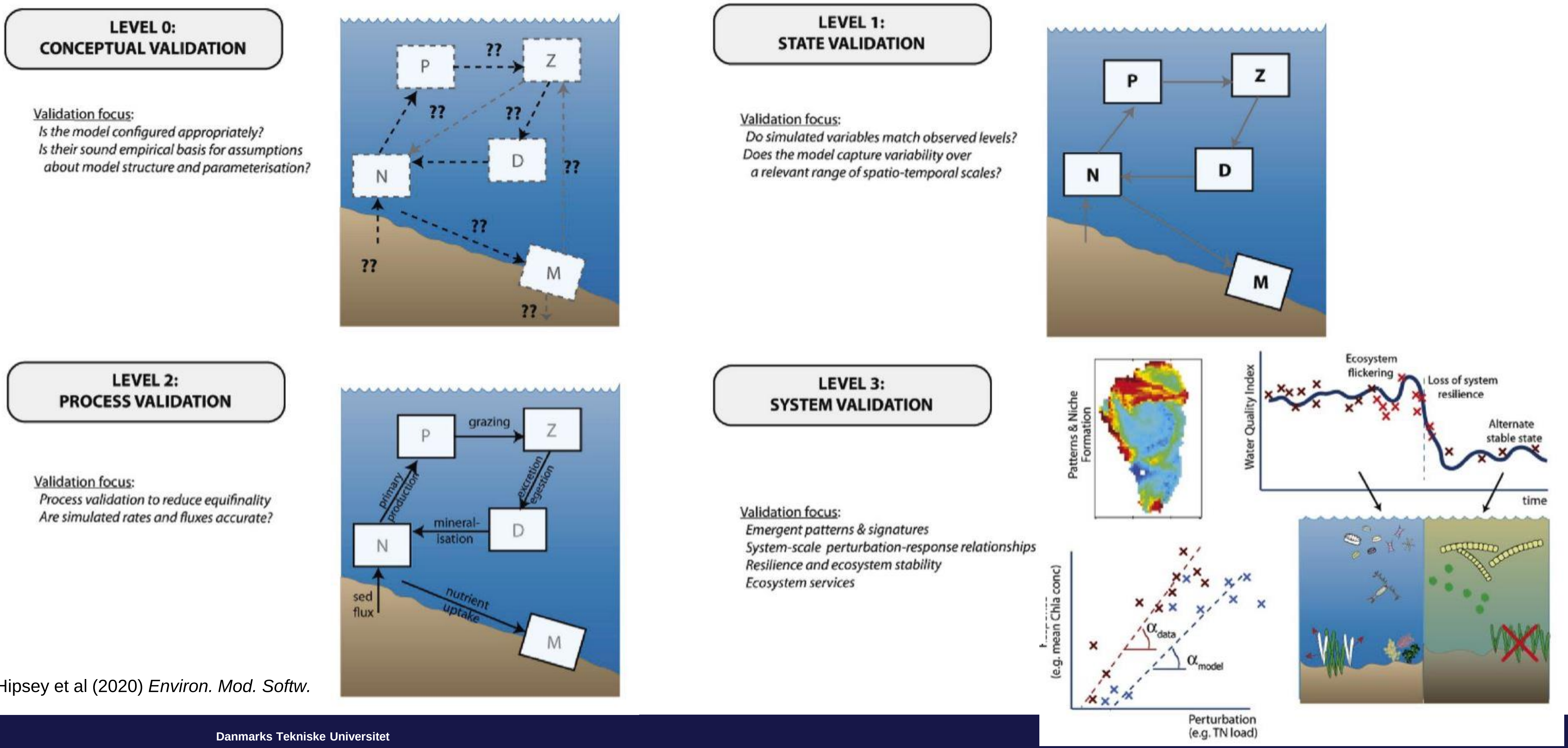
How do we best evaluate lake ecosystem models?



$$\frac{dN}{dt} = remineralization - N\ uptake$$



Beyond state variables: CSPC framework



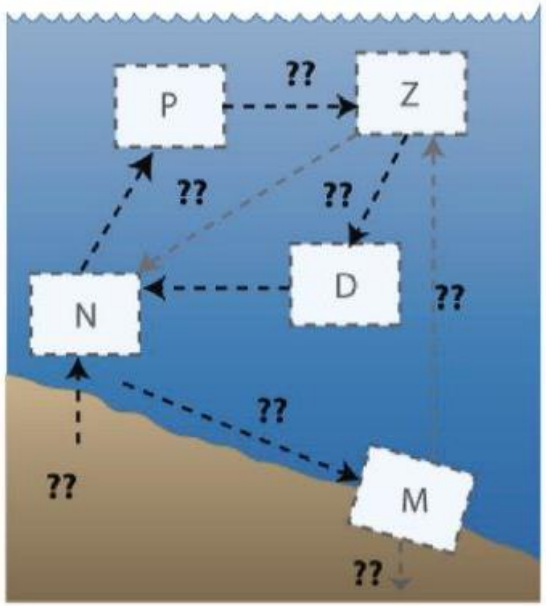
Hipsey et al (2020) *Environ. Mod. Softw.*

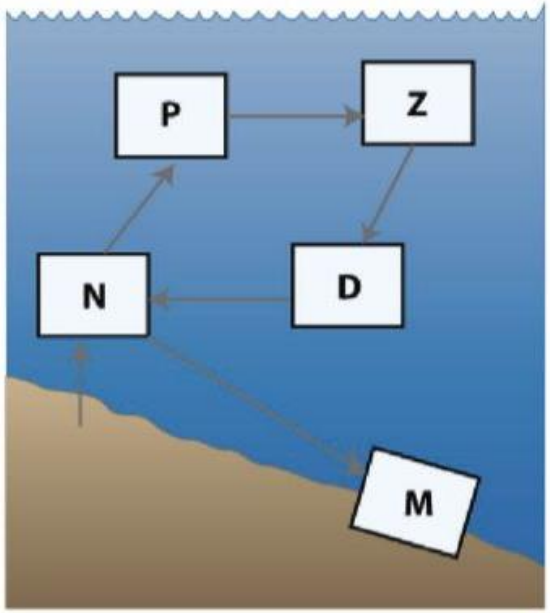
Beyond state variables: CSPC framework

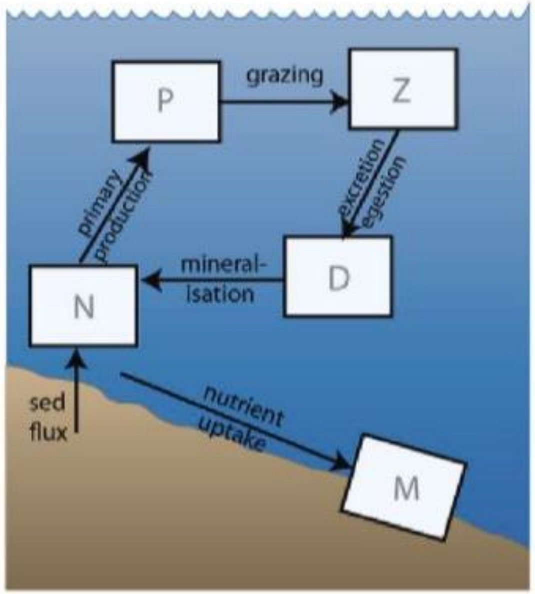
Structure → **Process** → **Function**

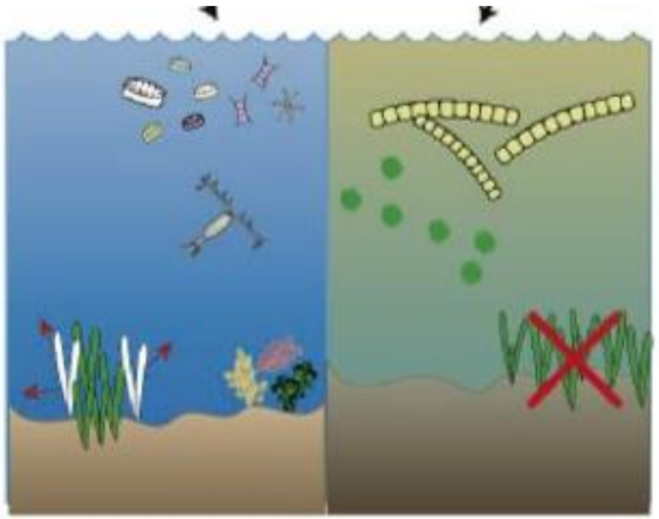
Improved predictability

Reduced uncertainty







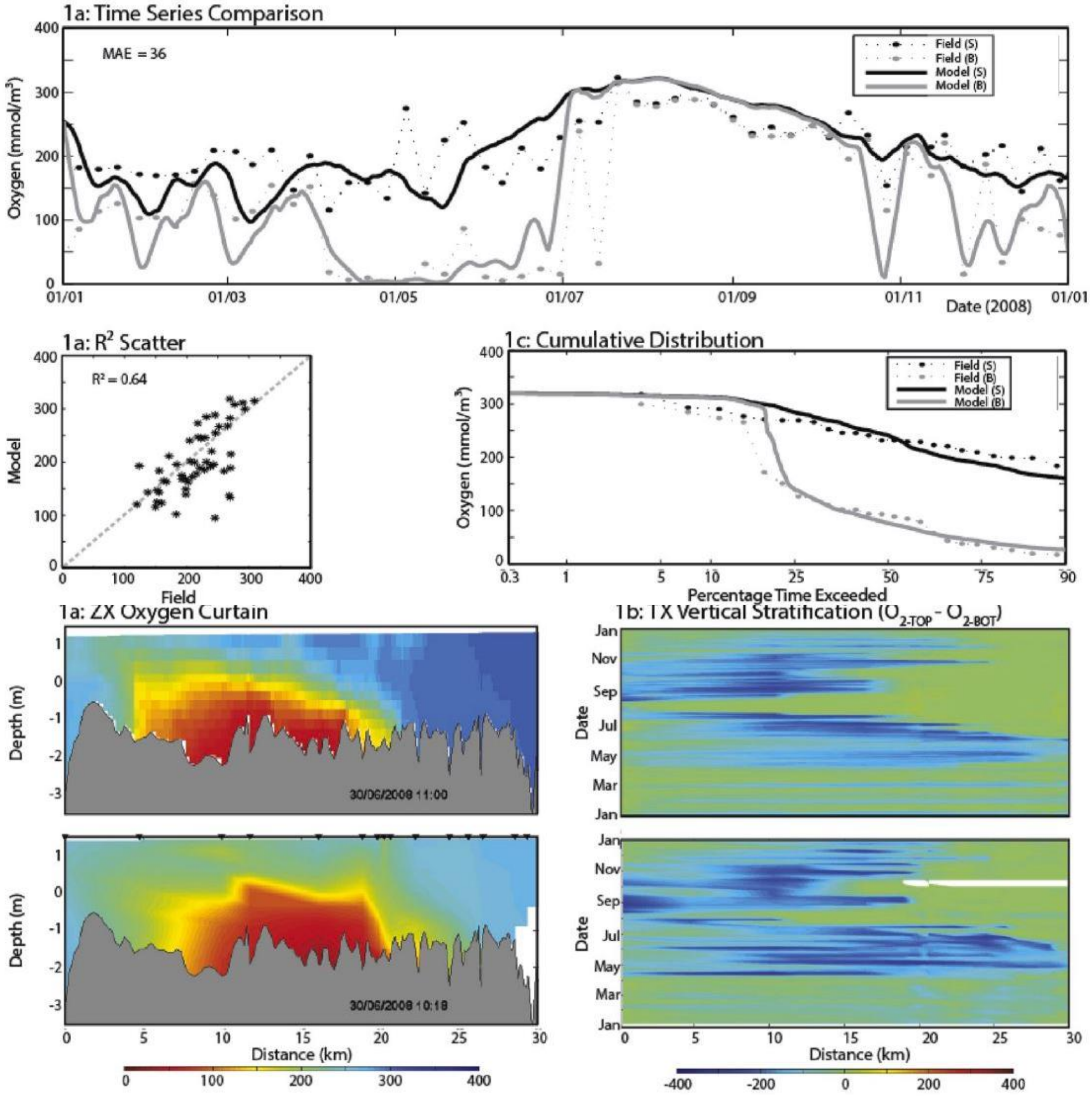


Level 0: **Conceptual** validation	Level 1: **State** validation	Level 2: **Process** validation	Level 2: **System** validation

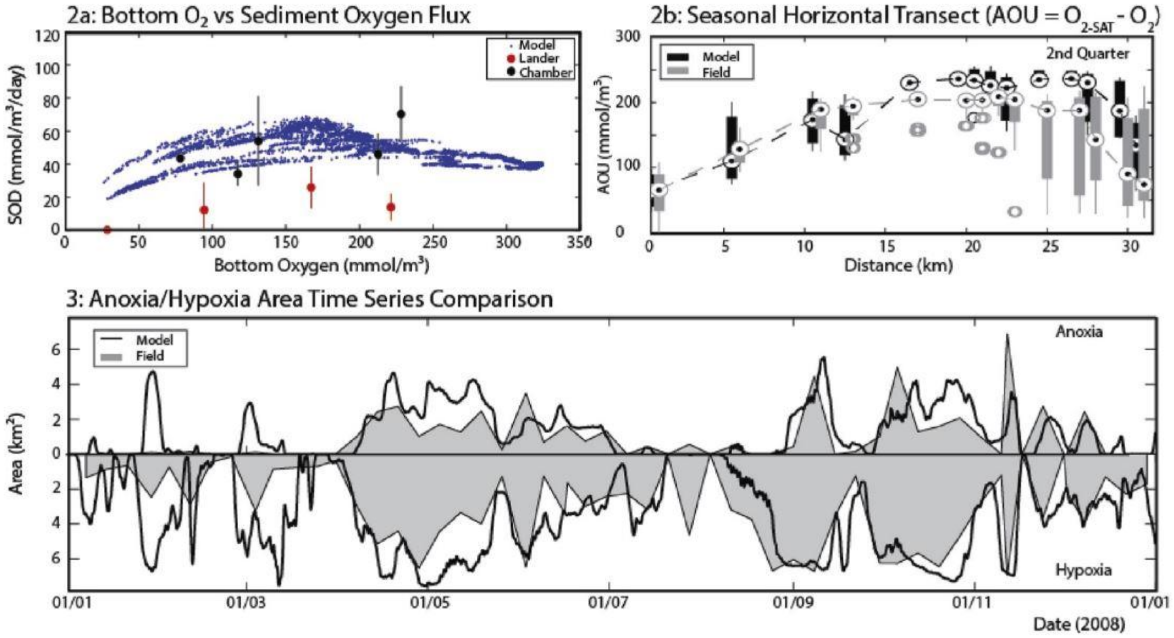
Hipsey et al (2020) *Environ. Mod. Softw.*

CSPS framework: an example

Level 1: State



Level 2: Process



Level 3: System

CSPS framework: a WET example

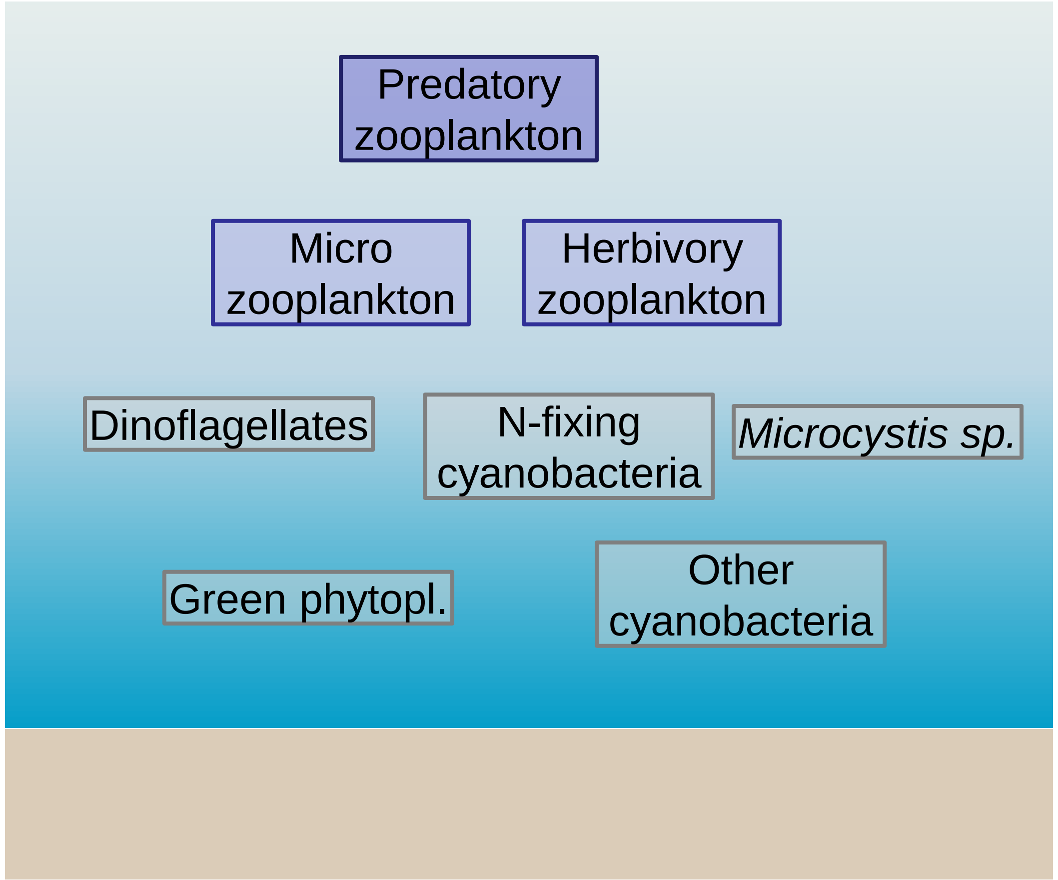
Regev, Carmel, Gal (2023)
Environ. Model. Softw.

Modelling Lake Kinneret (Sea of Galilee), a warm monomictic lake

Level 0: Conceptual

Table 3
Conceptual validation questions set forth by Hipsey et al. (2020) and responses.

Questions	Responses
(1) Conceptual representation	
(1 b) Does the model structure reflect recent advances in ecosystem understanding that may be important in this application?	Some ecosystem elements, such as anammox and dissimilative reduction of nitrate to ammonia (DRNA) processes (Madigan et al., 2012), were not incorporated in the WET model. Adding processes that we have little information about, will increase uncertainty. Also, simplicity was favored for accuracy.
(1c) Does the model reflect the system understanding of relevant local disciplinary experts and stakeholders?	Yes, the model setup was based on the DYRESM-CAEDYM setup (Gal et al., 2009) with some modification, and was build according to the decision makers questions and needs.



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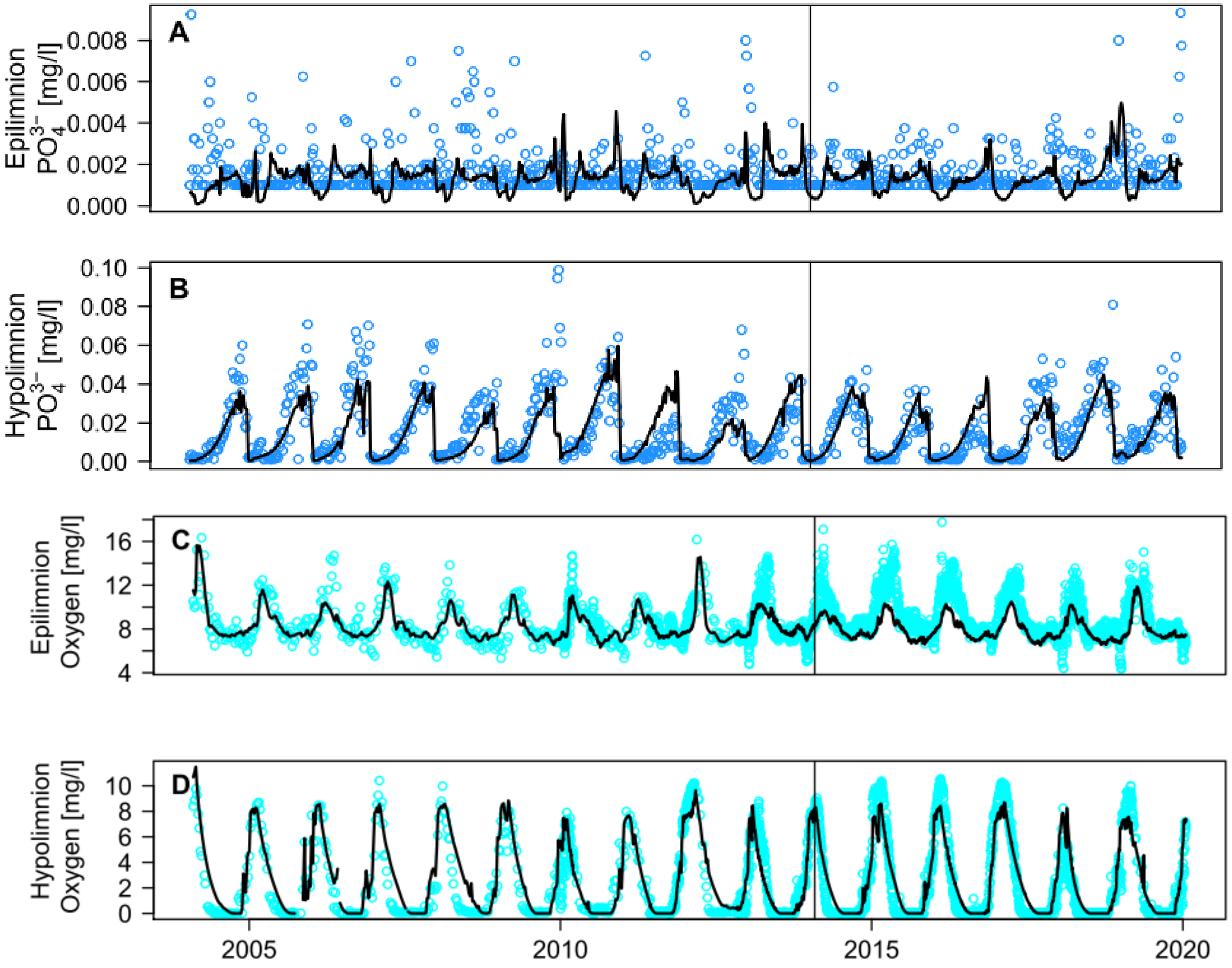
Level 1: State



CSPS framework: a WET example

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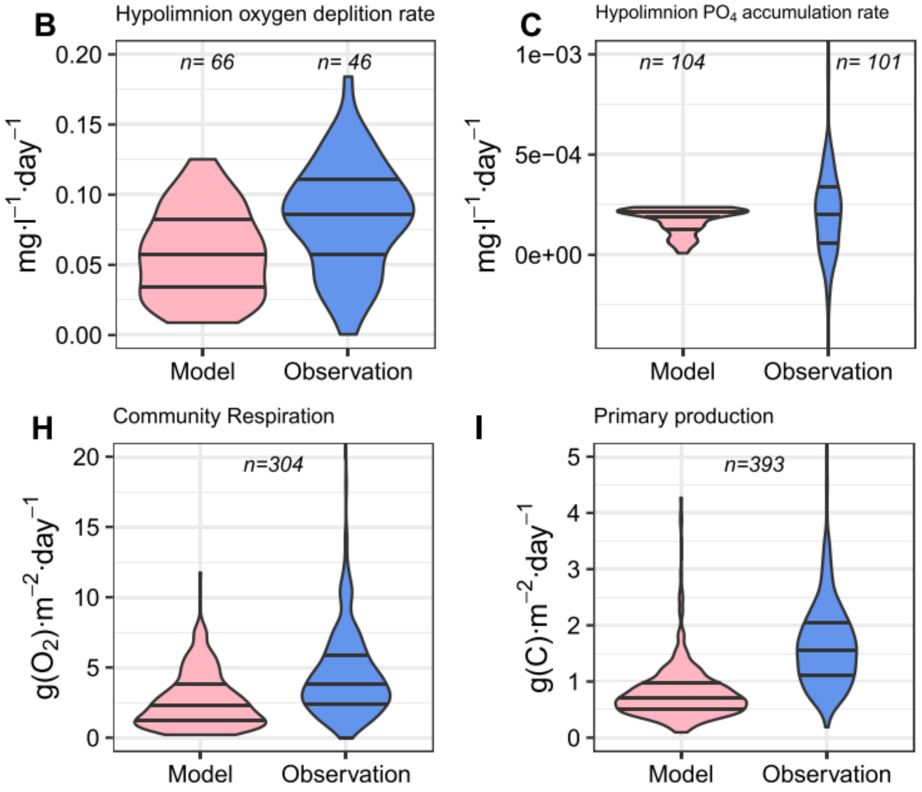
Level 2: Process



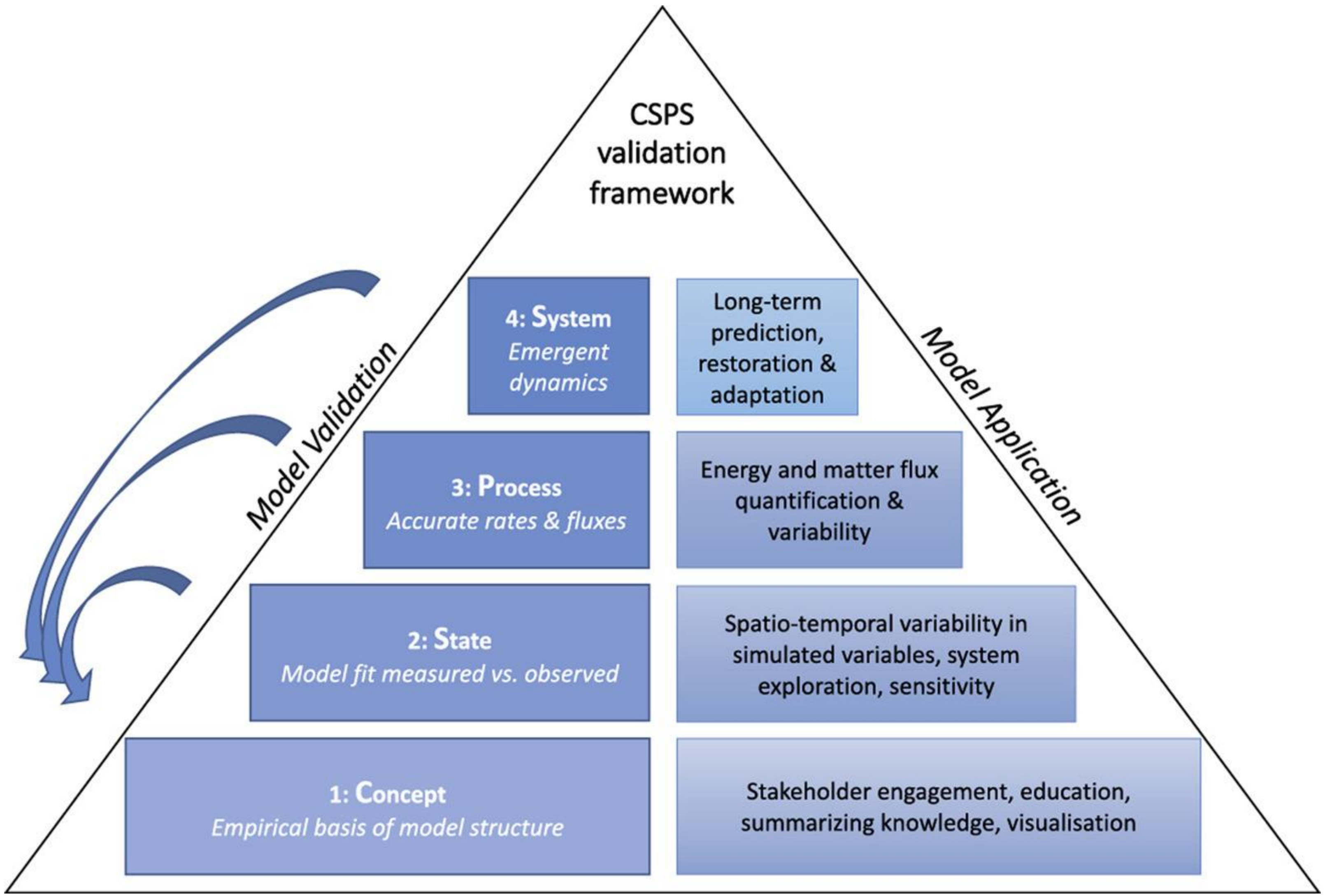
Level 3: System

Table 6

System Validation. R^2, P-val and slope of relation between variables in observation versus model. Based on epilimnion average monthly data, 30 years of observation and 16 years of model run. Abbreviation used: Tilda sign (~) denote linear relation tested between 2 variables; lvl_diff = lake level difference between consecutive months; NDOM/NPOM_Jordan = monthly mean of N dissolved/particulate organic matter concentration as measured in the Jordan stream multiplied by the flow expressed in [g/s]. In case a non-linear relation, the data were log transformed. Relations are interpreted as "agreement" if the linear model slope had same sign for both observation and model, and "disagreement" otherwise.

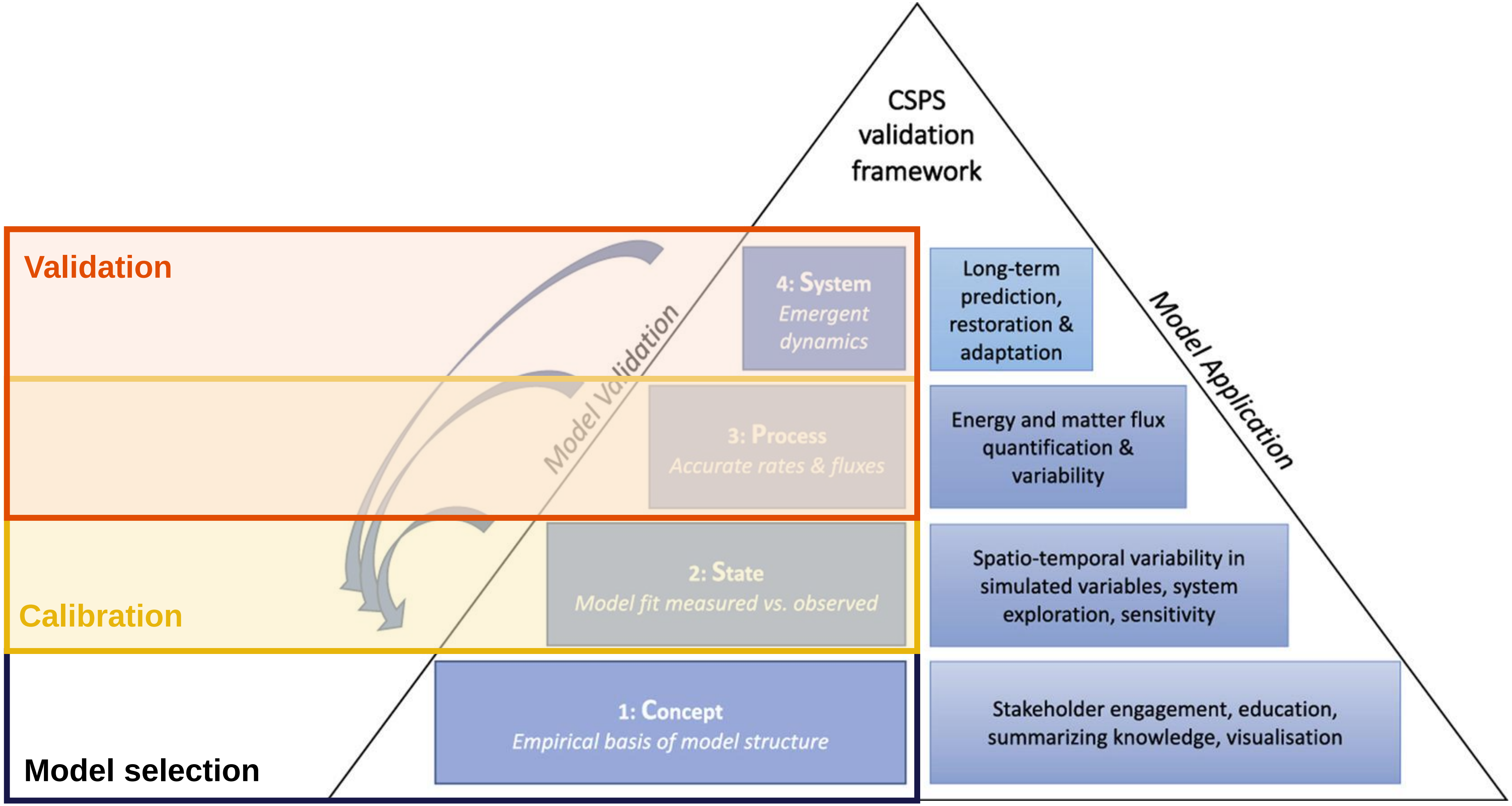
Relation	n		R^2		Slope		Results interpretation
	Obs	Model	Obs	Model	Obs	Model	
lvl_diff ~ NO_3^-	356	194	0.6	0.46	0.192	0.258	Agreement
Dino ~ NPOM	356	194	0.52	0.06	64	36	Agreement
lvl_diff ~ Temp	356	194	0.51	0.52	−0.048	−0.046	Agreement
lvl_diff1 ~ O_2	356	194	0.47	0.58	0.126	0.184	Agreement
lvl_diff ~ log(NfixCyano)	255	194	0.41	0.36	−0.082	−0.182	Agreement
MicroZoo ~ HerbZoo	356	194	0.39	0.21	0.293	−0.77	Disagreement
lvl_diff1 ~ log(Dino)	356	194	0.37	0.41	0.18	0.065	Agreement
log(Dino) ~ O_2	356	194	0.36	0.37	0.38	1.46	Agreement
log(NfixCyano) ~ log(NO_3^-)	255	194	0.35	0.39	−0.86	−1.11	Agreement
NO_3^- ~ O_2	356	194	0.35	0.16	0.44	0.268	Agreement
NO_3^- ~ NDOM_Jordan_mean	295	179	0.34	0.45	0.017	0.018	Agreement
log(NfixCyano) ~ Temp	255	194	0.32	0.58	0.283	0.16	Agreement
log(Dino) ~ log(NPOM_Jordan_mean)	340	181	0.29	0.43	0.66	2.2	Agreement
log(Dino) ~ log(NfixCyano)	255	194	0.28	0.05	−0.217	−0.69	Agreement
MicroZoo ~ PredZoo	356	194	0.26	0.74	1.58	1.05	Agreement

CSPS framework and model application



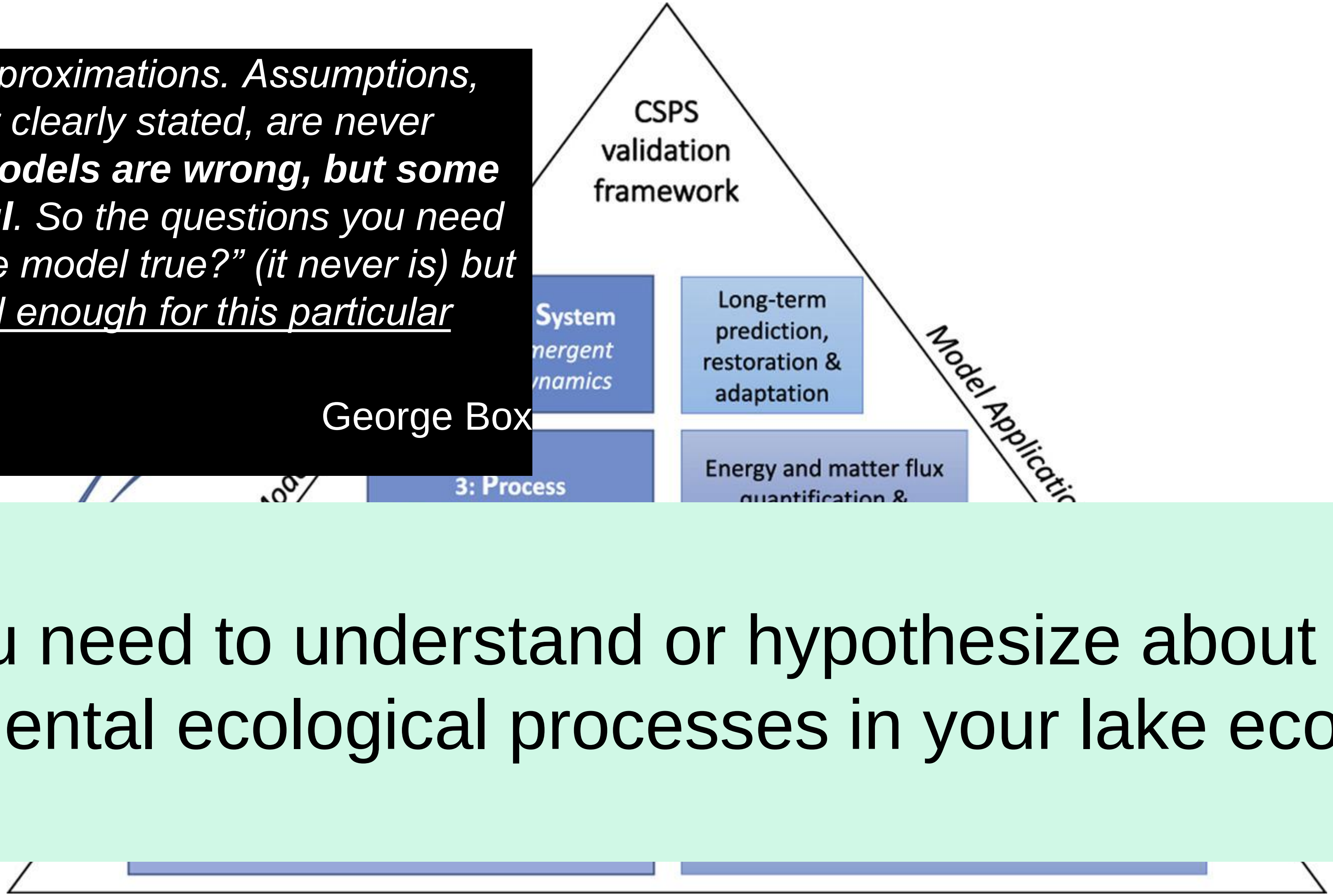
Hipsey et al (2020) *Environ. Mod. Softw.*

CSPS framework and calibration/validation



Hipsey et al (2020) *Environ. Mod. Softw.*

CSPS framework and model application



"All models are approximations. Assumptions, whether implied or clearly stated, are never exactly true. ***All models are wrong, but some models are useful****. So the questions you need to ask is not "Is the model true?" (it never is) but "Is the model good enough for this particular application?"*

George Box

You need to understand or hypothesize about the fundamental ecological processes in your lake ecosystem

Hipsey et al (2020) *Environ. Mod. Softw.*

Part III

Calibration strategy and process

CSPS framework and model application

1. Determine your model purpose
2. Decide on your lake food web configuration
3. Let the available data guide your calibration

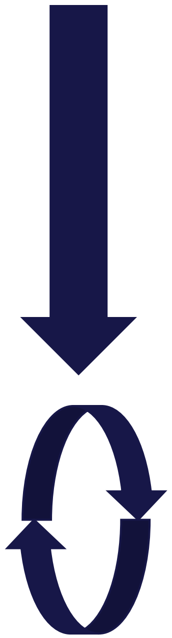
4. Calibration
   1. Determine parameters to include
   2. Determine relevant parameter value ranges

5. When is the calibration performance adequate?

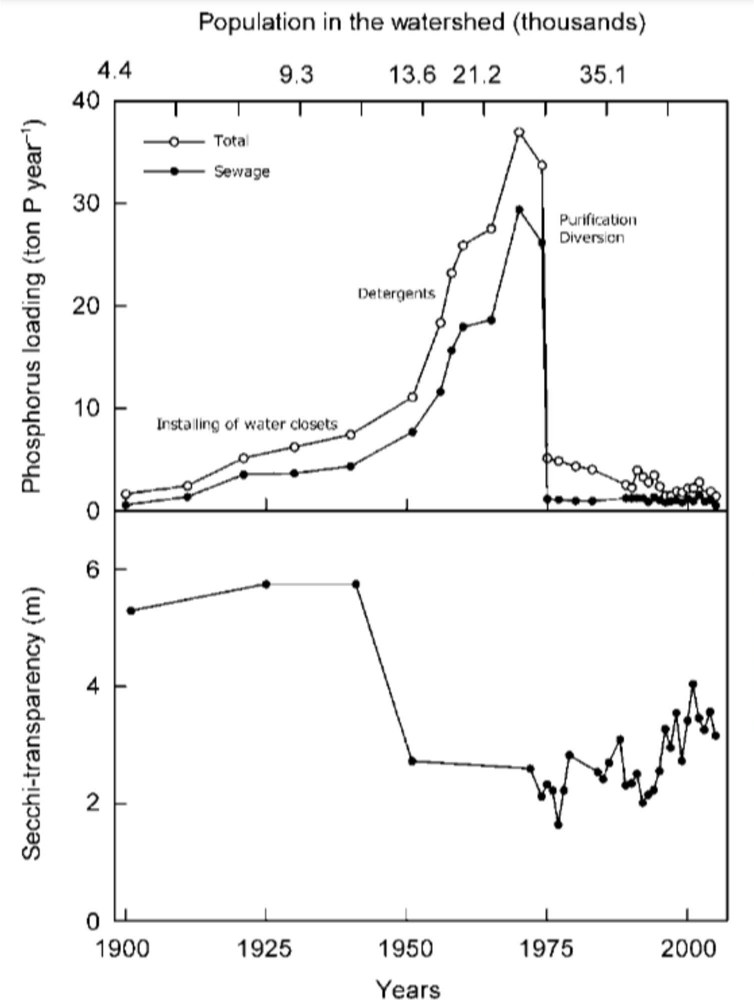
Next step: Validation

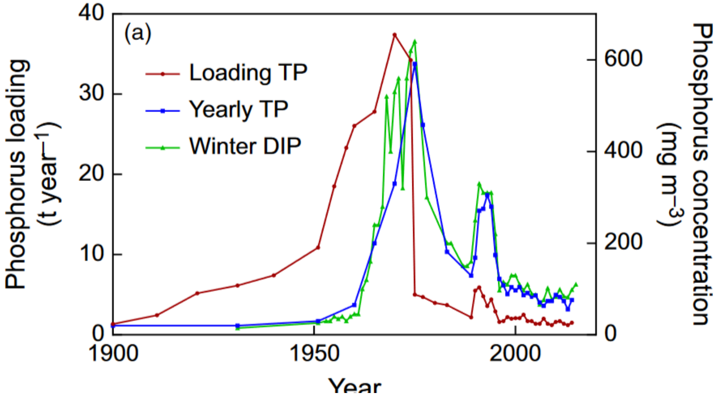
Calibration strategy for WET

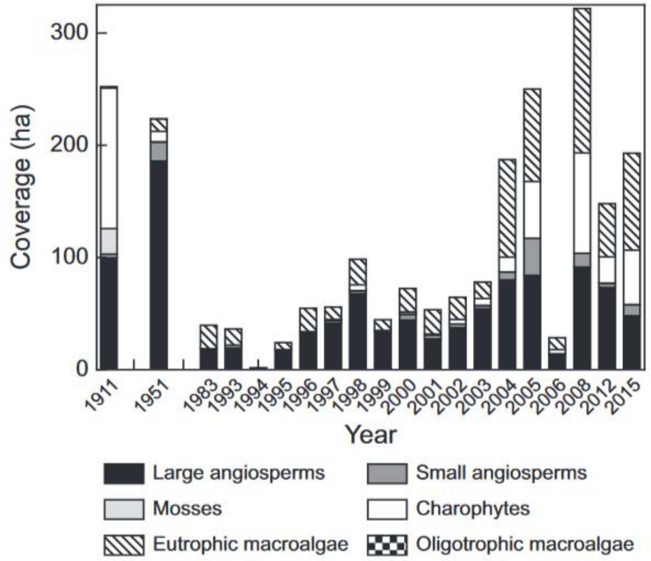
Step	Model focus	Processes	Observations
1	GOTM	Water column mixing	Water temperature
2	Metabolism	Decomposition and mineralization	Dissolved oxygen
3	Nitrogen	Denitrification and nitrification	NO_3 and NH_4
4	Phosphorous	P sediment release	PO4
5	Plankton	Nutrient uptake and grazing	TP, TN, Chl-a
6	Others		



Calibration strategy for WET: Lake Fure, an example







Calibration strategy for WET: Lake Fure, an example

Step	Model focus	Processes	Observations
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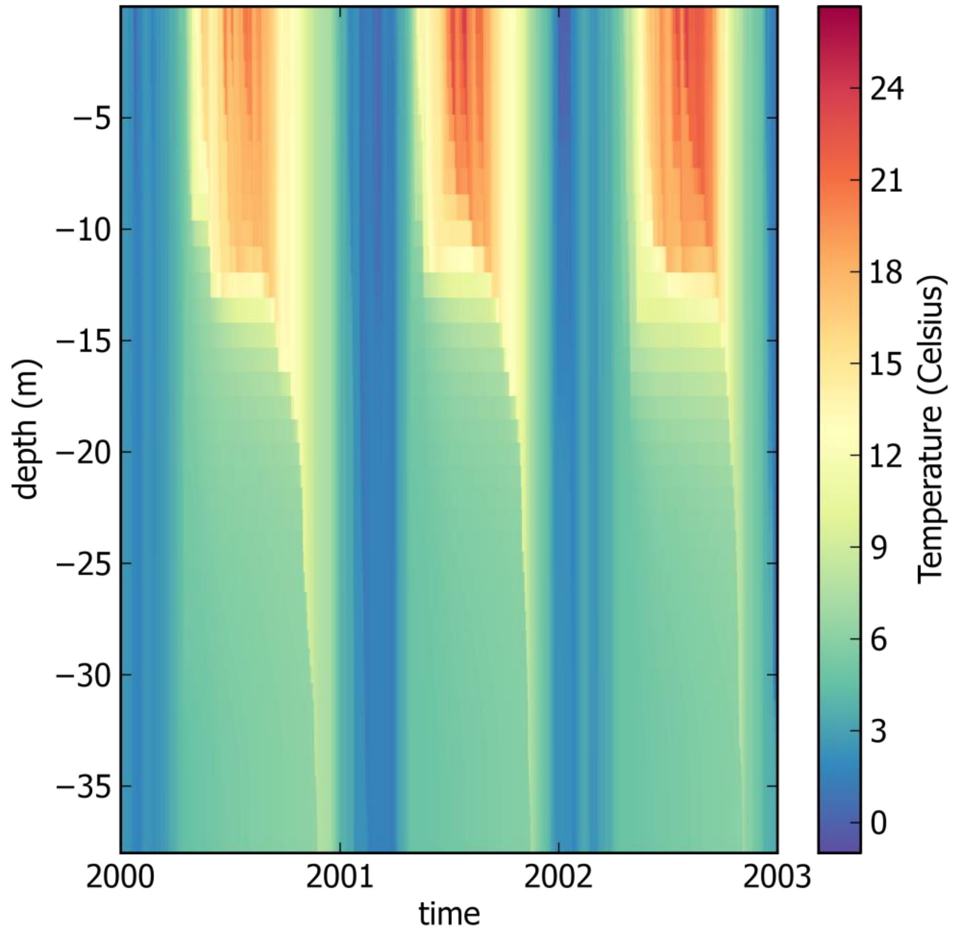

Calibration strategy for WET: Lake Fure, an example

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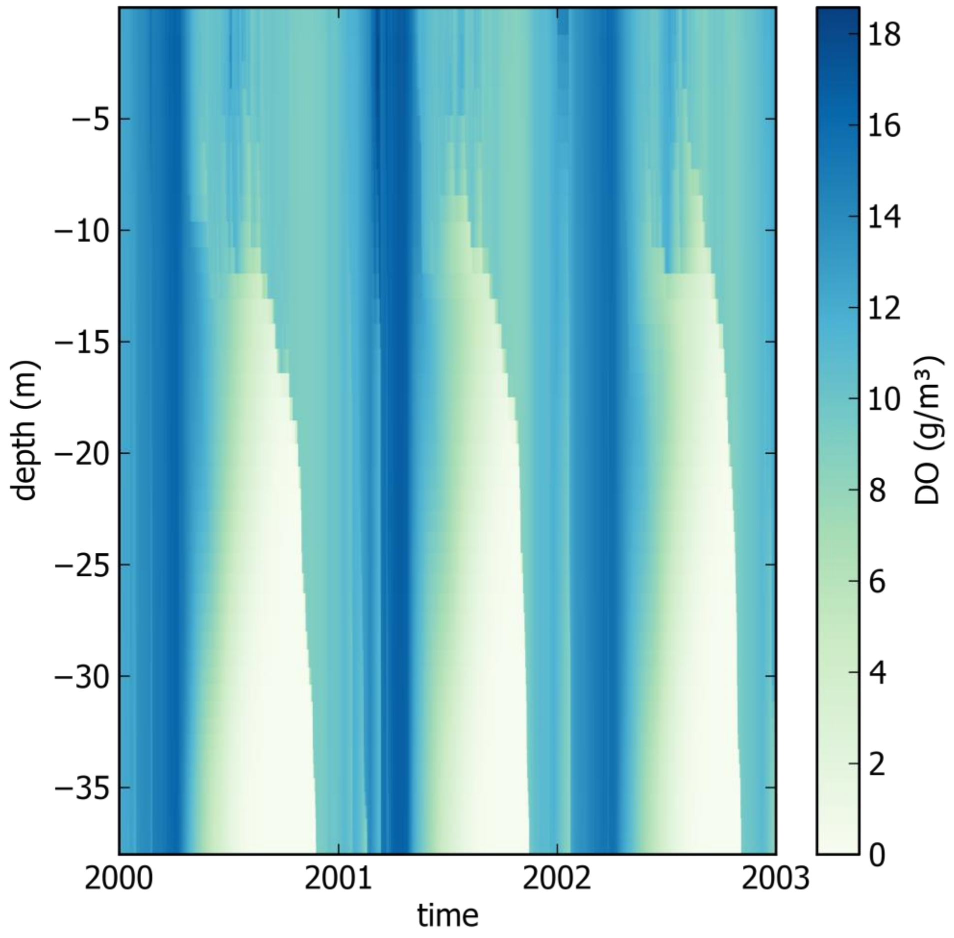

Calibration strategy for WET: Lake Fure, an example

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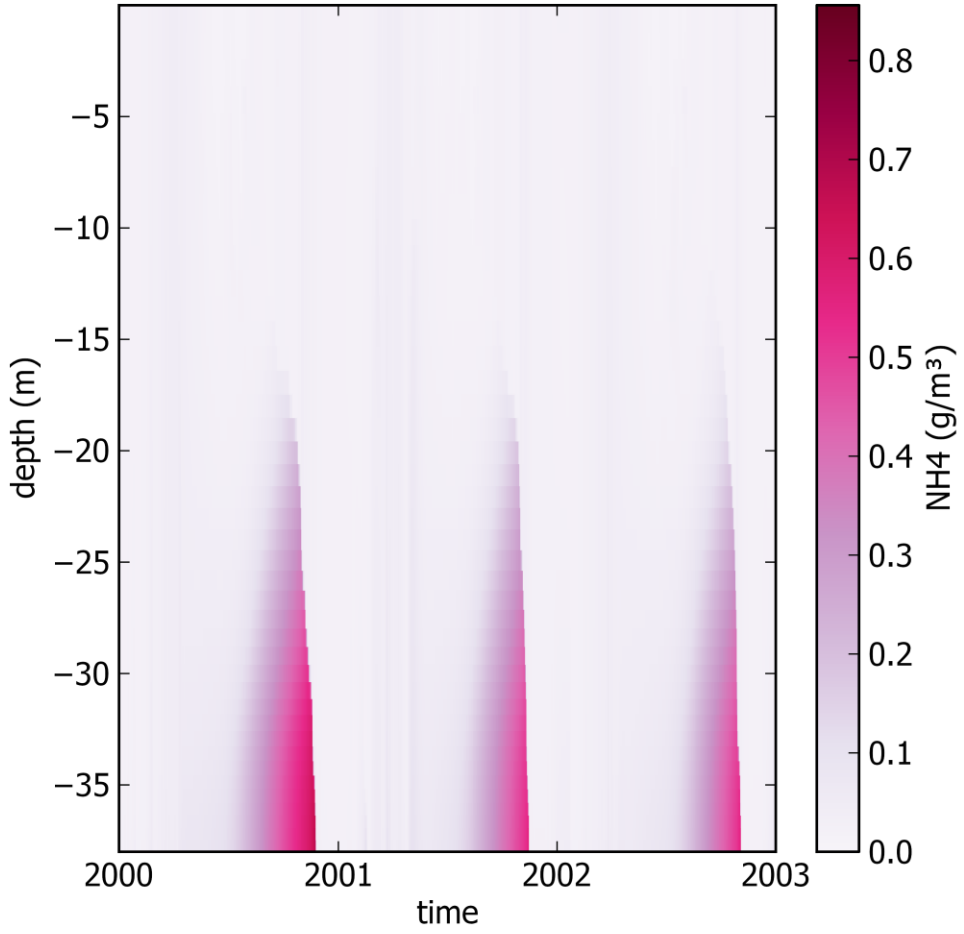

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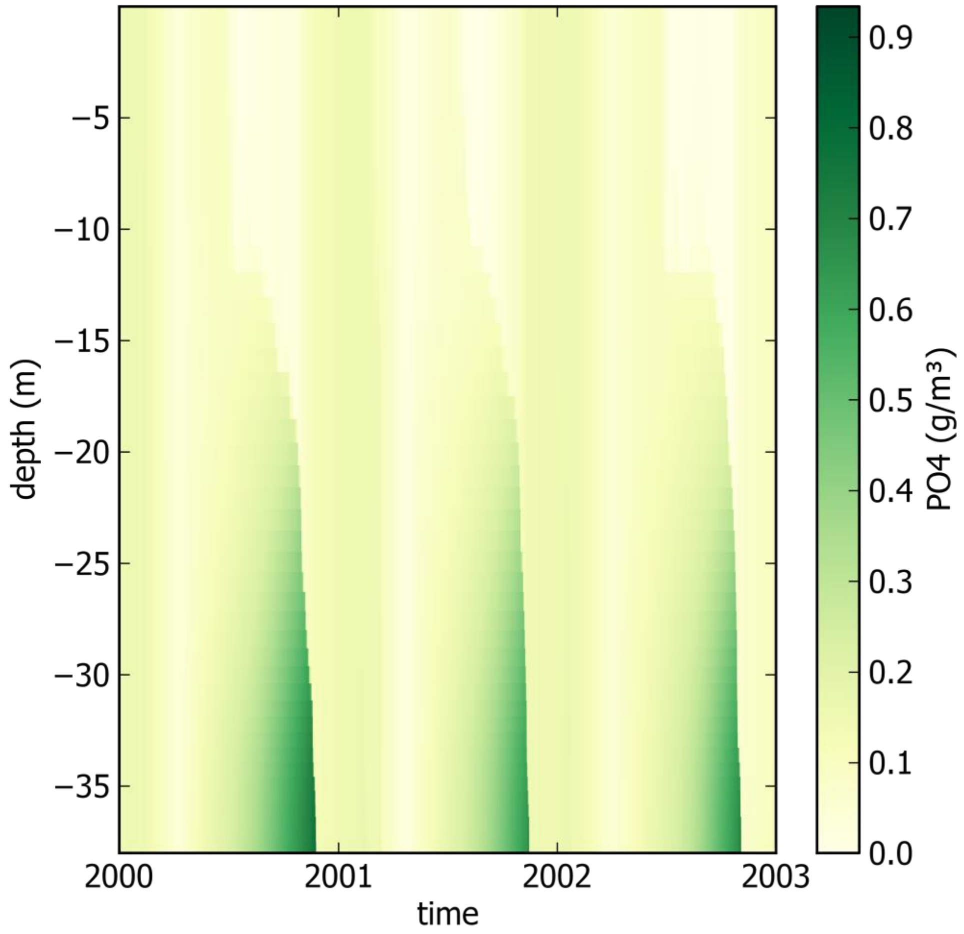

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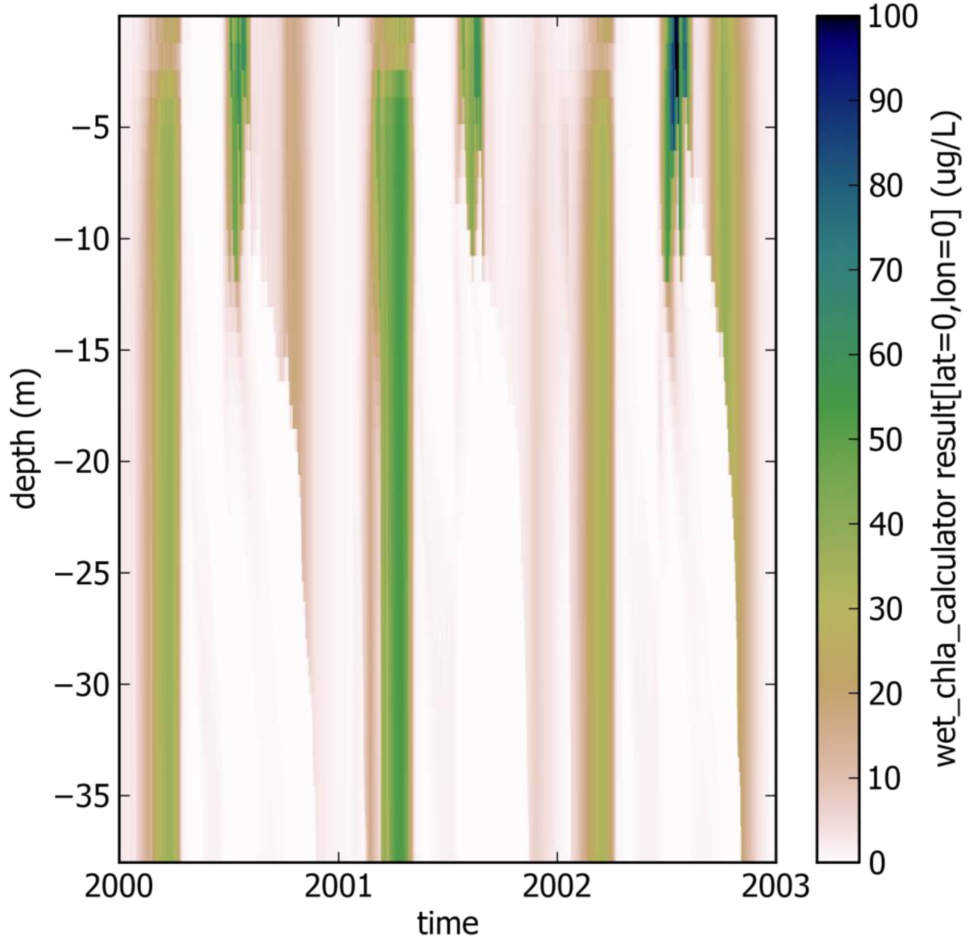

Calibration strategy for WET: Lake Fure, an example

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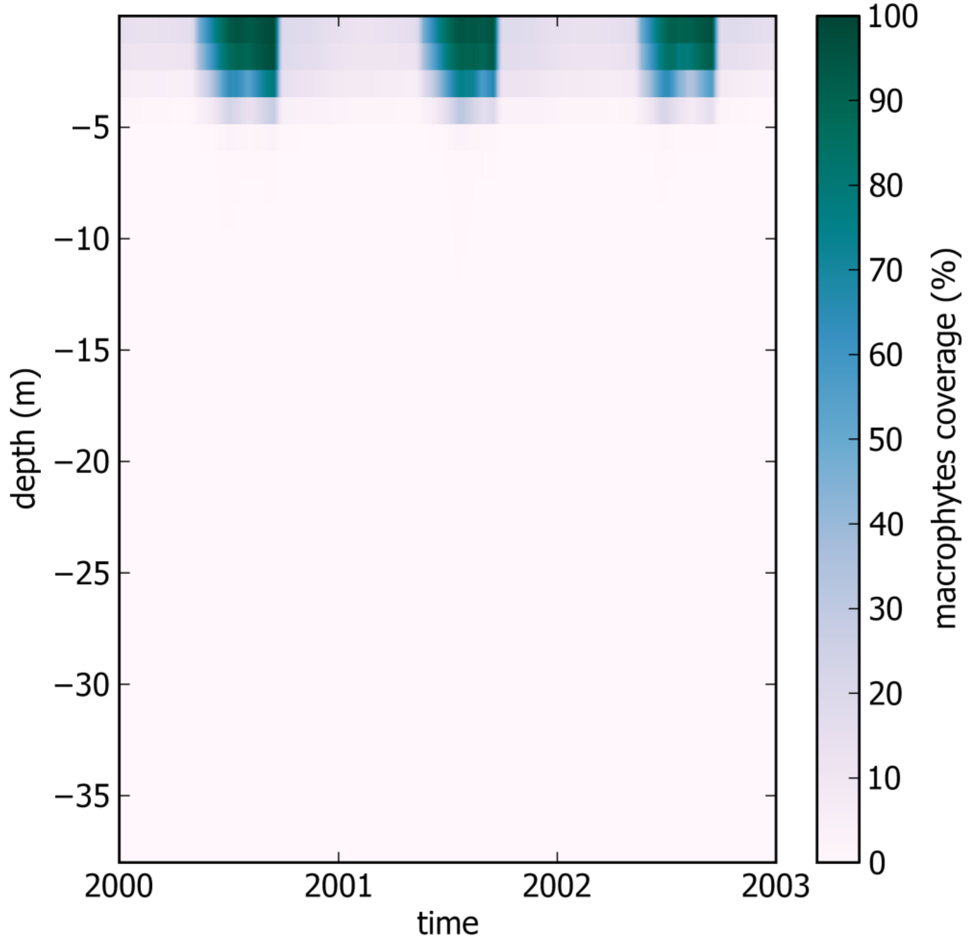
6	**Vegetation**	**Macrophyte growth**	**Vegetation coverage**

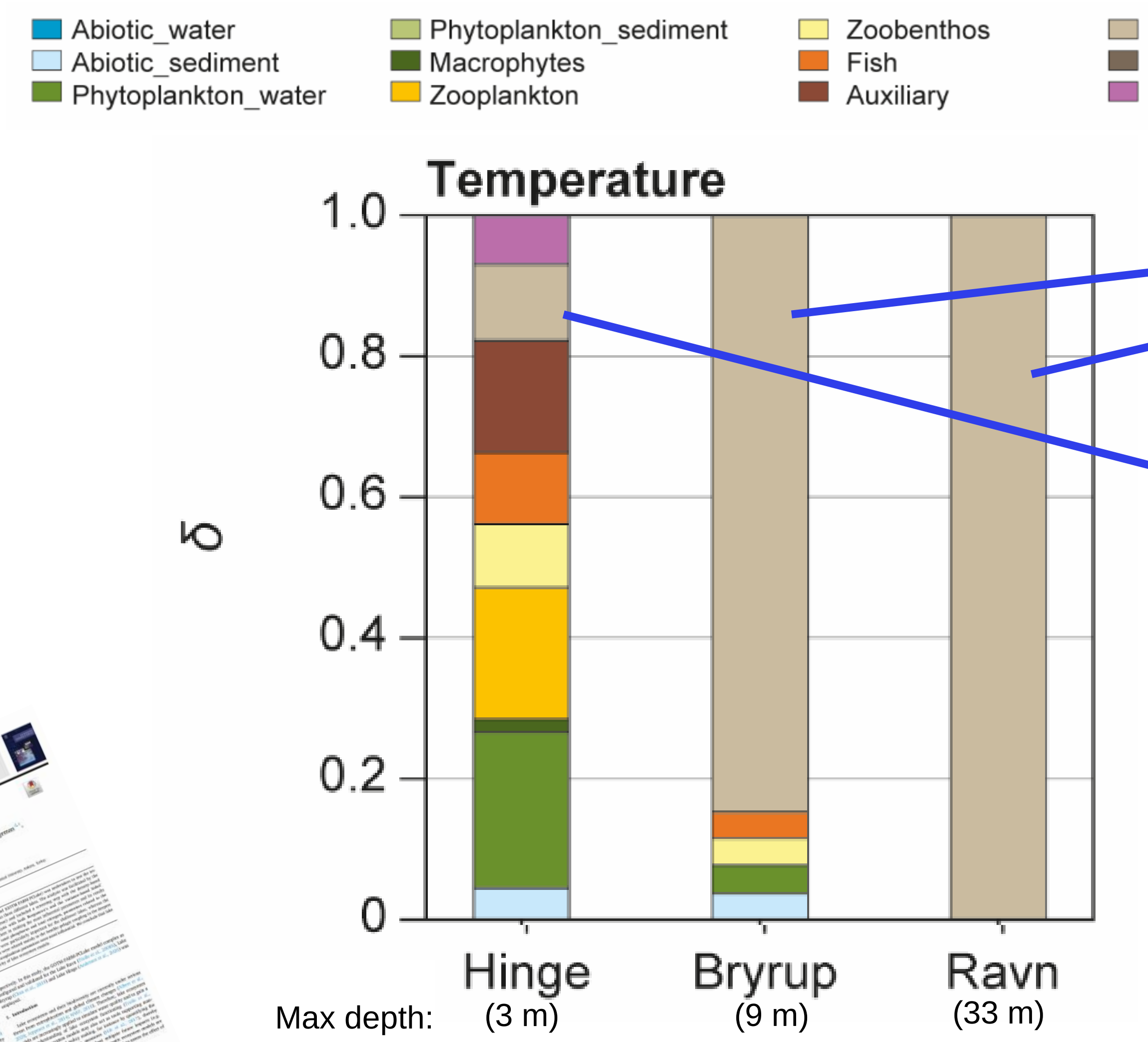


Selecting important model parameters

To gather information on which parameters to include in your calibration, you should search for

- Sensitivity studies with GOTM, FABM-PCLake and WET
- Model papers with GOTM, FABM-PCLake and WET
- User experiences

Selecting important model parameters



- **wind_factor (GOTM)**
- Factor to scale observed wind speed (in *meteo_file*)

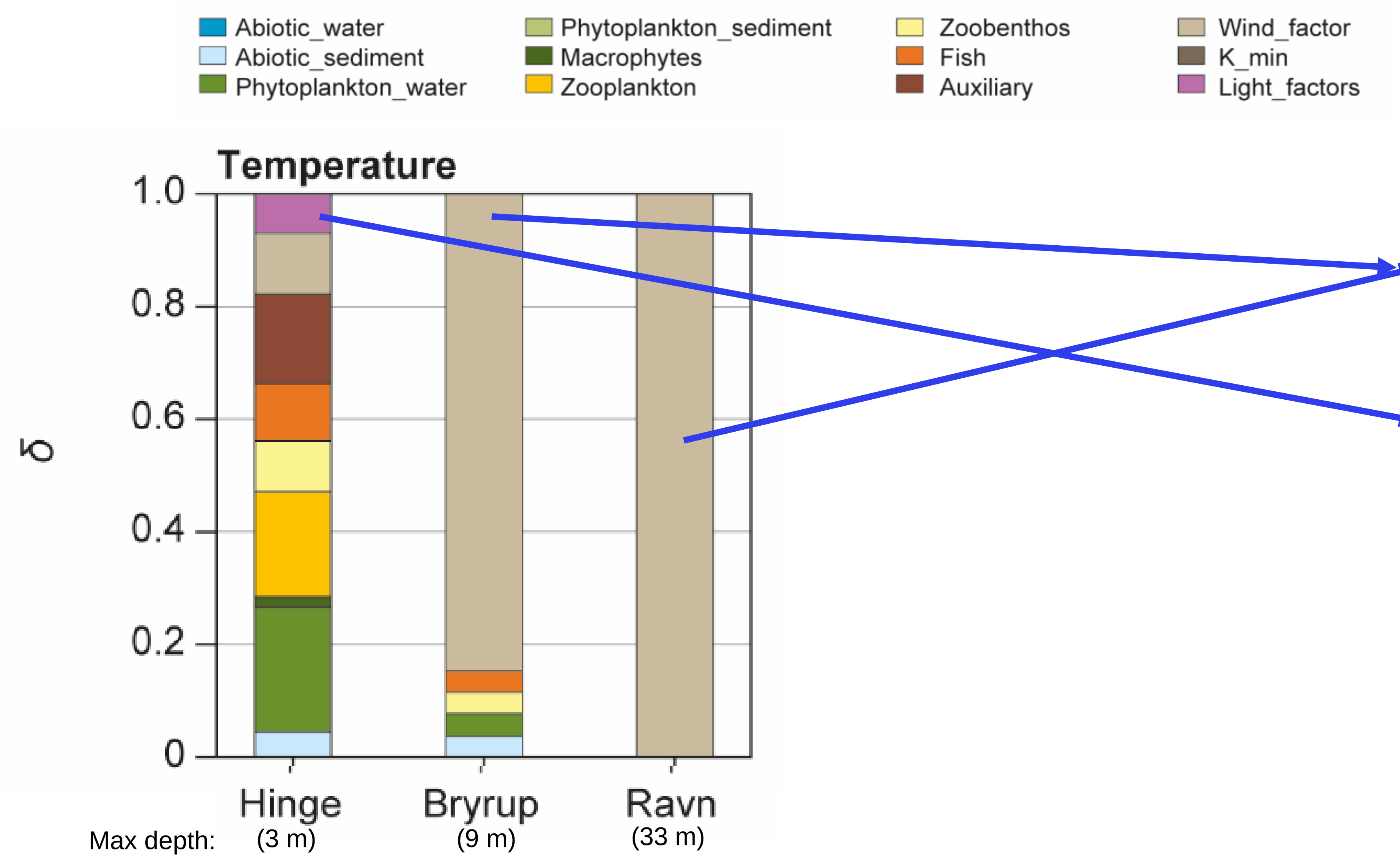
- **A, g1, g2 (GOTM)**
- Light extinction coefficients

- Concentration of particles can also be important in simulating light conditions and therefore also temperature.

Andersen et al. (2020) *How morphology shapes the parameter sensitivity of lake ecosystem models*

Selecting important model parameters

Andersen et al. (2020) *How morphology shapes the parameter sensitivity of lake ecosystem models*



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Selecting important model parameters

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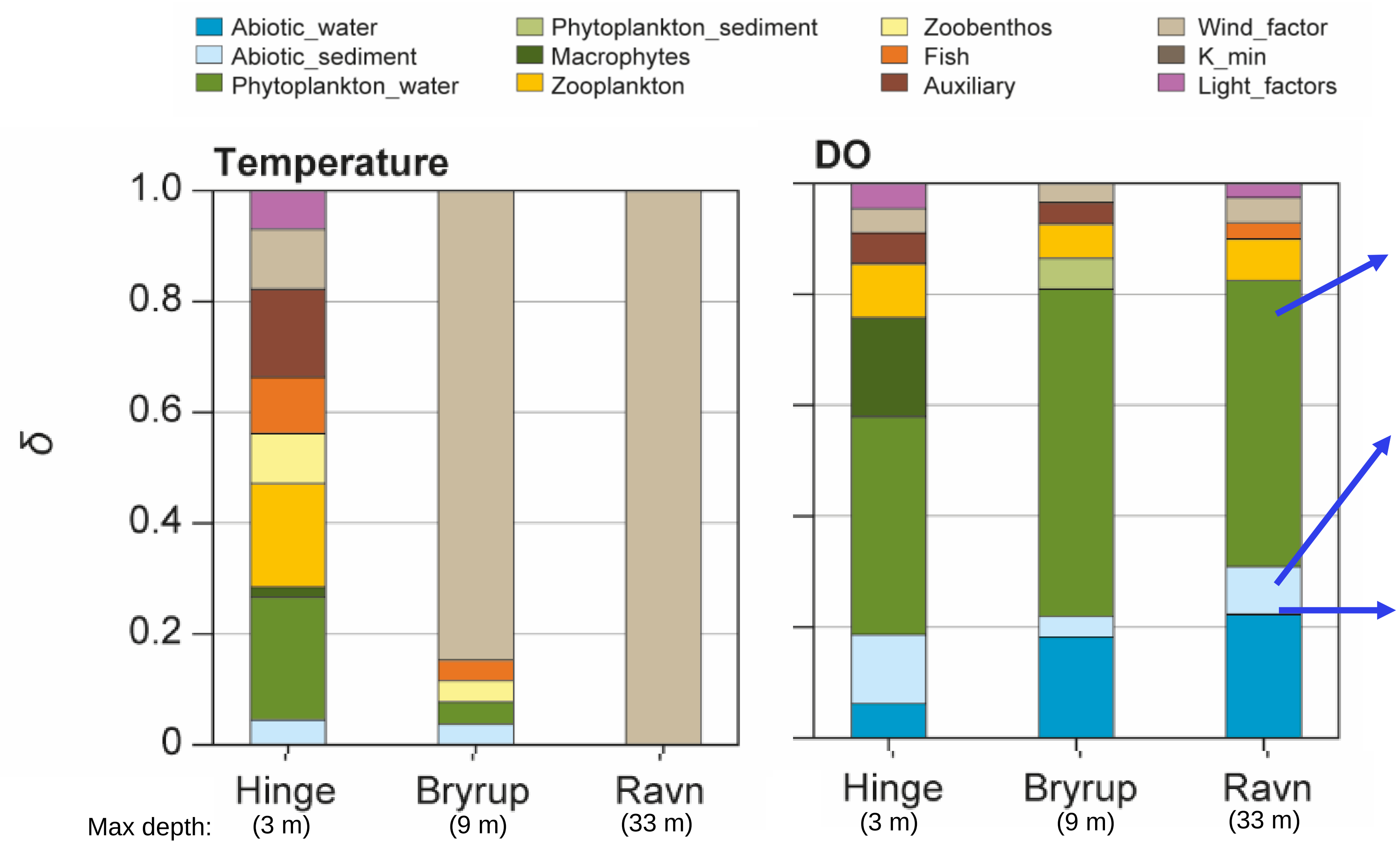

- **cMuMaxPhyto (WET)**
- Growth rate of phytoplankton groups

- **kDMinPOMS (WET)**
- Decomposition rate of POM-DW at 20*C

- **cThetaMinPOMS (WET)**
- Temperature coefficient of POM decomposition

Selecting important model parameters from SA

Subset of SA results from Andersen et al (2020) for Lake Ravn mean summer total chlorophyll a concentration:

Total chl-a											
cleaned						cleaned_sub1					
Parameter_name	**S1**	**S1_conf**	**delta**	**delta_conf**	**module**	**Parameter_name**	**S1**	**S1_conf**	**delta**	**delta_conf**	**module**
cFiltMax	0.199	0.008	0.168	0.0039	zooplankton	cFiltMax	0.2	0.0083	0.169	0.0045	zooplankton
cTmOptZoo	0.087	0.0059	0.115	0.0039	zooplankton	cTmOptZoo	0.087	0.0058	0.115	0.004	zooplankton
fDAssZoo	0.085	0.0056	0.097	0.0039	zooplankton	fDAssZoo	0.084	0.0059	0.097	0.0043	zooplankton
cPrefBlue	0.076	0.005	0.096	0.0039	zooplankton	cPrefBlue	0.076	0.0048	0.096	0.0044	zooplankton
cSigTmZoo	0.053	0.0046	0.086	0.0039	zooplankton	cSigTmZoo	0.053	0.0046	0.085	0.0041	zooplankton
cMuMaxBlue	0.044	0.0045	0.082	0.0041	phytoplankton_water	cMuMaxBlue	0.044	0.0041	0.083	0.004	phytoplankton_water

Selecting important model parameters from SA

Subset of SA results from UPDATED TO WET v2.1 for Lake Ravn mean summer total chlorophyll a concentration:

Total chl-a											
cleaned						cleaned_sub1					
Parameter_name	S1	S1_conf	delta	delta_conf	module	Parameter_name	S1	S1_conf	delta	delta_conf	module
kDConsMaxZoo	0.199	0.008	0.168	0.0039	zooplankton	kDConsMaxZoo	0.2	0.0083	0.169	0.0045	zooplankton
cTMOptZoo	0.087	0.0059	0.115	0.0039	zooplankton	cTMOptZoo	0.087	0.0058	0.115	0.004	zooplankton
fDAssZoo	0.085	0.0056	0.097	0.0039	zooplankton	fDAssZoo	0.084	0.0059	0.097	0.0043	zooplankton
------------------	0.076	0.005	0.096	0.0039	zooplankton	------------------	0.076	0.0048	0.096	0.0044	zooplankton
cSigTmZoo	0.053	0.0046	0.086	0.0039	zooplankton	cSigTmZoo	0.053	0.0046	0.085	0.0041	zooplankton
cMuMax	0.044	0.0045	0.082	0.0041	phytoplankton_water	cMuMax	0.044	0.0041	0.083	0.004	phytoplankton_water

NOTE: Some parameters have changed name from FABM-PCLake to WET v2.1.

If you cannot find parameter in fabm.yaml, it has likely been removed or renamed.

For instance, fish and zooplankton feeding parameters e.g. preference factors for phytoplankton (e.g. cPrefBlue) has been replaced with feeding parameters documented in Schnedler-Meyer & Andersen (2024, paper on WET v2.1).

Understanding the ecosystem = Build parameter library

To understand your case study and to reproduce the ecosystem as best as possible with your model, you should **leverage as many relevant information sources as possible**, for instance scientific publications, reports or data sets/sources etc.

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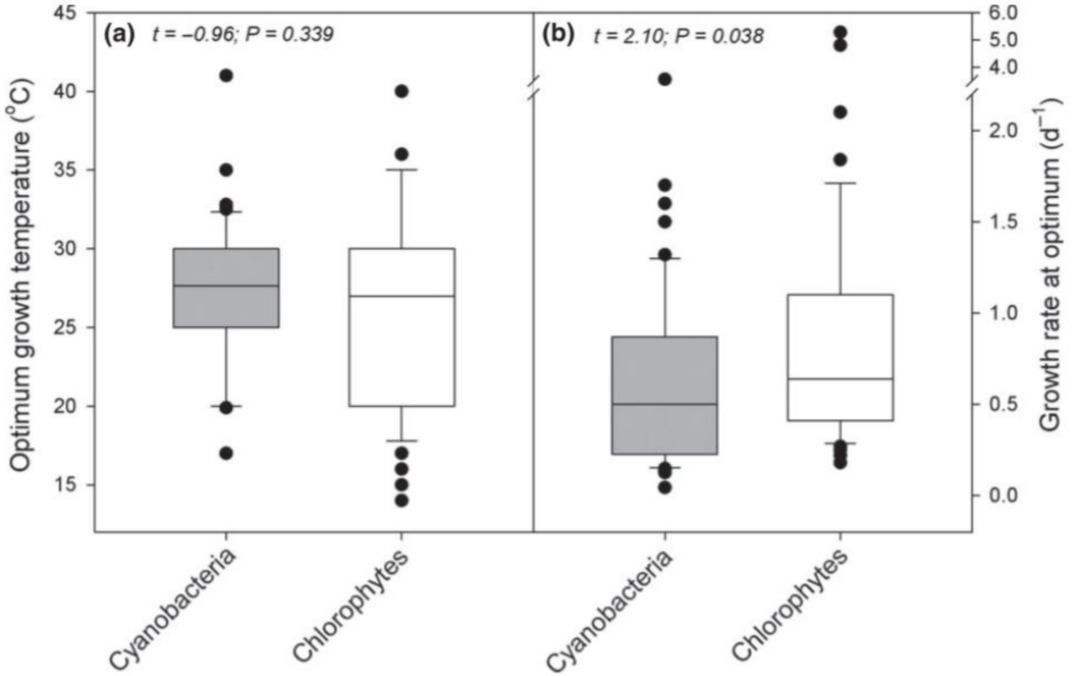
Table 3. The mean decomposition rates of the various organic phosphorus fractions for different decomposition models. The units of the decomposition rates are day^{-1}.

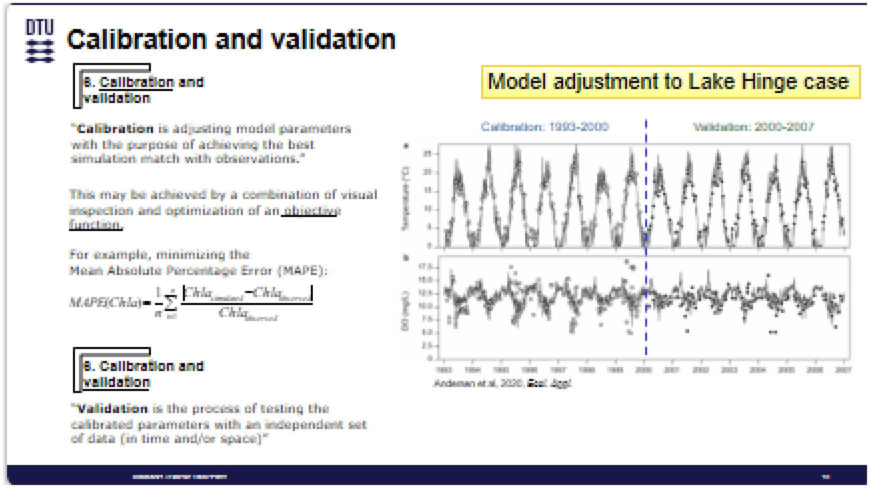
	Models and rate coefficients						
	TOP → DIP	POP → DIP	POP → DOP → DIP		LPOP → LDOP → DIP		
Rivers	k_{TOP}	k_{POP1}	k_{POP2}	k_{DOP2}	k_{LPOP}	k_{LDOP}	n
North Han	0.034	0.031	0.031	0.302	0.123	0.485	30
South Han	0.038	0.056	0.057	0.426	0.130	1.035	27
Lower Han	0.050	0.071	0.063	0.448	0.178	0.680	6
Kum	0.034	0.046	0.043	0.294	0.146	0.818	25
Youngsan	0.036	0.049	0.042	0.255	0.174	0.670	32
Sumjin	0.035	0.035	0.038	0.244	0.143	0.622	32
Mean (SD)	0.038 (0.006)	0.048 (0.013)	0.046 (0.011)	0.328 (0.080)	0.149 (0.021)	0.718 (0.172)	152

Islam et al. (2012). The decomposition rates of organic phosphorus and organic nitrogen in river waters. Freshwater Biology

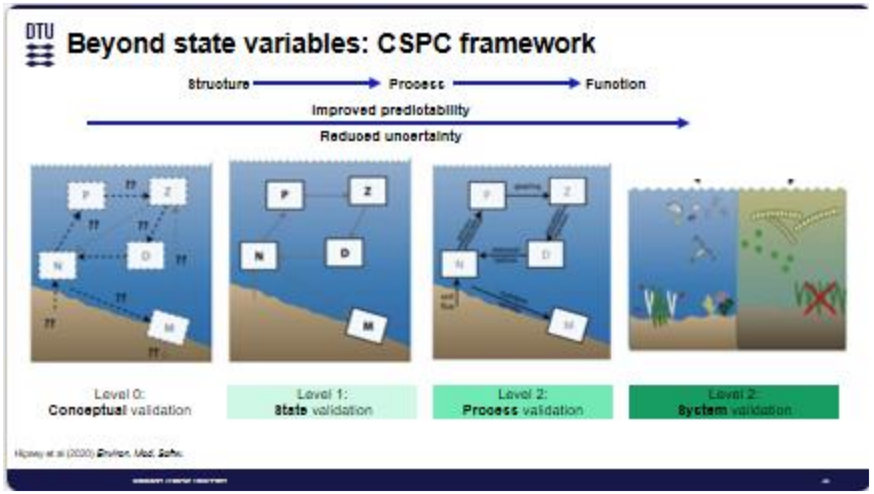


Lürling et al. (2013). Comparison of cyanobacterial and green algal growth rates at different temperatures. Freshwater Biology, *58*(3), 552–559.

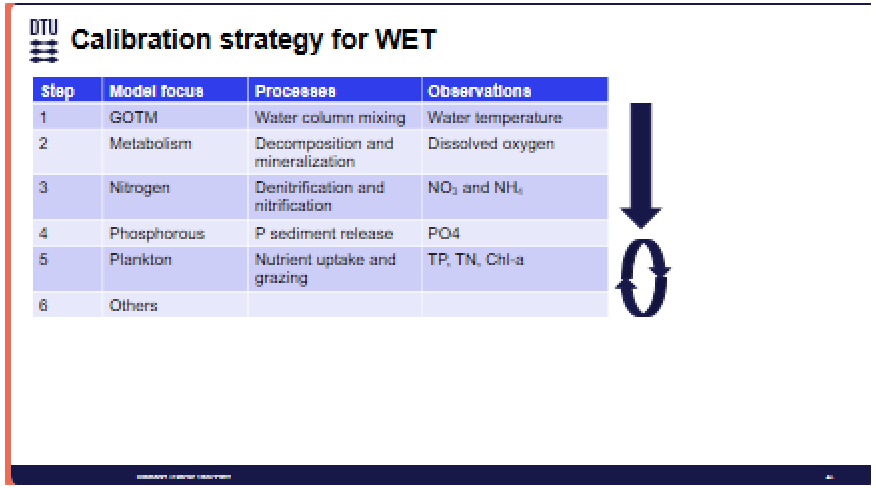
Take aways



Calibration and validation
8. Calibration and validation
Model adjustment to Lake Hinge case
"Calibration is adjusting model parameters with the purpose of achieving the best simulation match with observations."
This may be achieved by a combination of visual inspection and optimization of an objective function.
For example, minimizing the Mean Absolute Percentage Error (MAPE):
Calibration: 1993-2000
Validation: 2000-2007
8. Calibration and validation
"Validation is the process of testing the calibrated parameters with an independent set of data (in time and/or space)"



Beyond state variables: CSPC framework
Structure
Process
Function
Improved predictability
Reduced uncertainty
Level 0: Conceptual validation
Level 1: State validation
Level 2: Process validation
Level 2: System validation



Calibration strategy for WET
Step
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GOTM
Water column mixing
Water temperature
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Decomposition and mineralization
Dissolved oxygen
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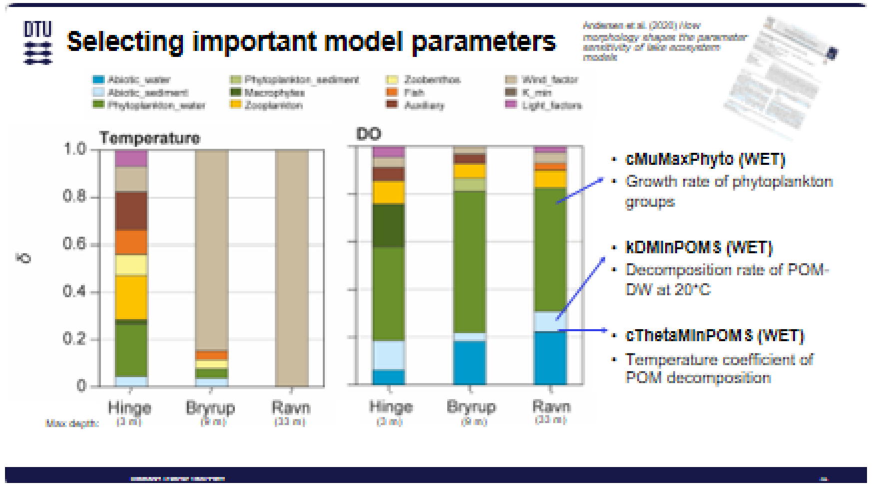

Selecting important model parameters
Temperature
DO
Hinge
Bryrup
Ravn
cMuMaxPhyto (WET)
Growth rate of phytoplankton groups
kDMinPOMS (WET)
Decomposition rate of POM-DW at 20°C
cThetaMinPOMS (WET)
Temperature coefficient of POM decomposition