Analysis of the transferability of a biogeochemical lake model to lakes of different trophic state

Johanna Mieleitner

Department of Systems Analysis, Integrated Assessment and Modelling (SIAM)
Swiss Federal Institute of Environmental Science and Technology (EAWAG)
8600 Dübendorf, Switzerland

Contents

Motivation

- Goal of lake modelling
  - Predictive power and transferability
  - Correct mechanistic description
- Problem
  - Lake models lack predictive power and transferability
- Question
  - Can the transferability be increased by
    - Changing the model formulation?
    - Changing the parameter values?

Goals

- Test transferability
  - Find a minimum subset of parameters with different values for different lakes
- Improve the understanding of the causes of the need for lake specific calibration
- Improve universality
  - Of the model parameter values
  - Of the model structure

Case Study

- Lakes under similar climatic conditions with different trophic state
  - Walensee (oligotrophic)
  - Lake Zürich (mesotrophic)
  - Greifensee (eutrophic)
- Application of the lake model developed by Omlin et. al 2001 to the three lakes

Lakes and Data

Lakes

Watersheds

Rivers

Measurement Points (▲)

Waste water treatment plants (•)

Model Overview

Physical Part:

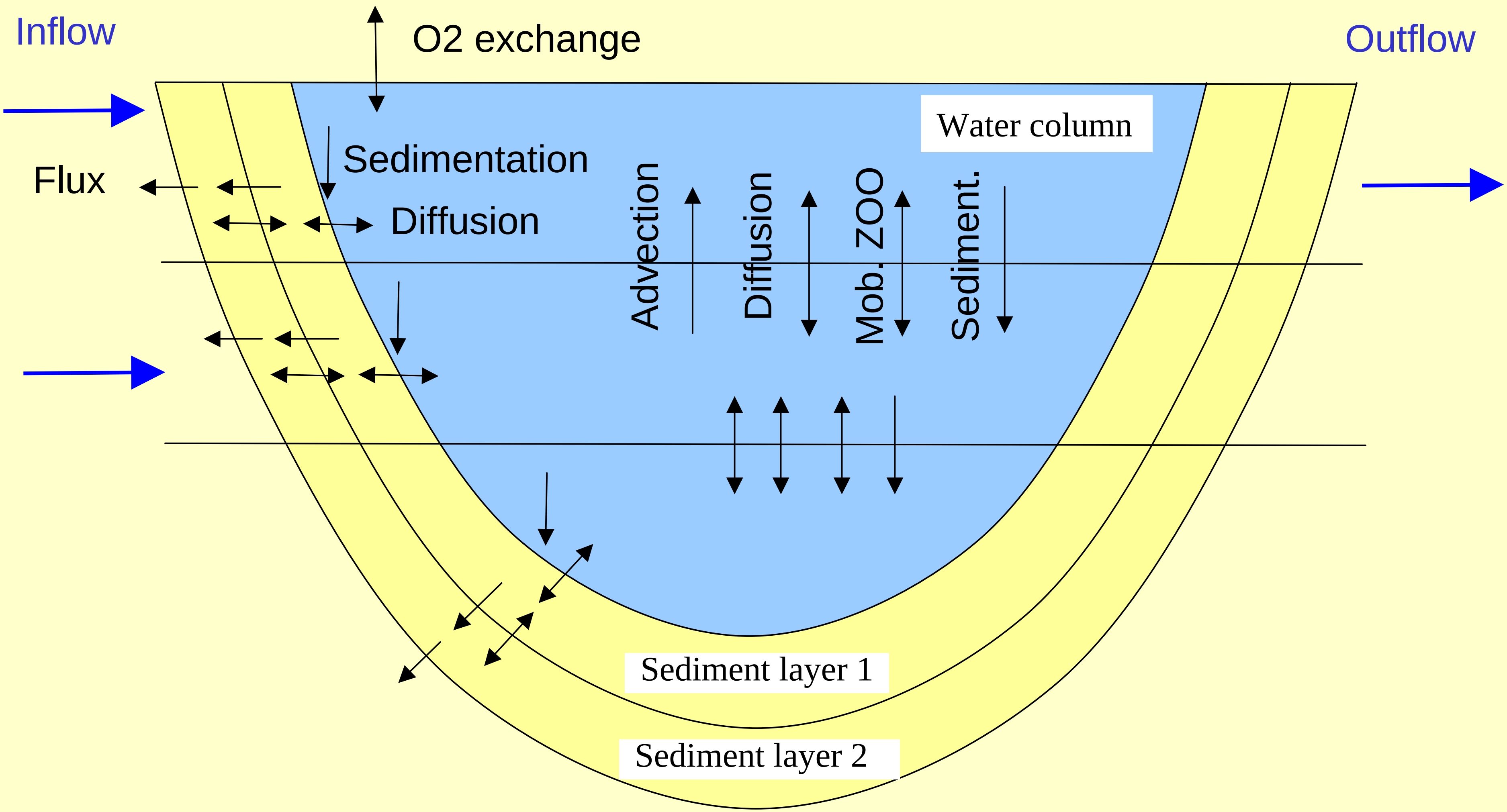
- One dimensional (resolving the depth of the lake)
- Horizontally mixed

Biochemical Part:

- Substances: Algae, Zooplankton, PO_4, NH_4, NO_3, O_2, degradable and inert organic particles
- Transformation processes

Implementation with AQUASIM

Model (AQUASIM Lake Comp.)



Model: Stoichiometry Matrix

		Substances											
		S_{NH4}	S_{NO3}	S_{HPO4}	S_{O2}	X_{ALG}	$X_{P,ALG}$	X_{ZOO}	X_S	$X_{P,S}$	$X_{PI,S}$	X_I	$X_{P,I}$
		gN/m³	gN/m³	gP/m³	gO/m³	gDM/m³	gP/m^3	gDM/m³	gDM/m3	gP/m³	gP/m³	gDM/m3	gP/m³
Processes	**Gro ALG NO3**		$-a_N$	$-b_P$	1.2	1	b_P						
	Growth ALG NH4	$-a_N$		$-b_P$	0.93	1	b_P						
	Gro ZOO	$\nu_{ZOO,N}$		$\nu_{ZOO,P}$	$-\nu_{ZOO,O}$	$-1/Y_{ZOO}$	$-a_{P,ALG}/Y_{ZOO}$	1	f_e/Y_{ZOO}	0			
	Resp ALG	a_N		$a_{P,ALG}$	-0.94	-1	$-a_{P,ALG}$						
	Resp ZOO	a_N		$a_{P,red}$	-0.94			-1					
	Death ALG					-1	$-a_{P,ALG}$		1-fp	$(1-f_p)a_{P,ALG}$		fp	$f_p\ a_{P,ALG}$
	Death ZOO							-1	1-fp	$(1-f_p)a_{P,red}$		fp	$f_p\ a_{P,red}$
	Death ZOO Dipt							-1	1-fp	$(1-f_p)a_{P,red}$		fp	$f_p\ a_{P,red}$
	Aer miner	a_N		$a_{P,S}+a_{PI,S}$	-0.94				-1	$-a_{P,S}$	$-a_{PI,S}$		
	Anox miner	a_N	-0.33	$a_{P,S}+a_{PI,S}$					-1	$-a_{P,S}$	$-a_{PI,S}$		
	Anae miner	a_N		$a_{P,S}+a_{PI,S}$					-1	$-a_{P,S}$	$-a_{PI,S}$		
	Nitrification	-1	1		-4.6								
	P-Uptake			-1							1		

Model: Process Rates

Nr.	Process	Rate
1	Growth ALG NO3	$k_{gro,ALG,T0} \cdot \exp(\beta_{ALG}(T-T_0)) \cdot \frac{I(z)}{K_{I,ALG}+I(z)} \cdot \min\left(\frac{S_{NO3}+S_{NH4}}{K_{N,ALG}+S_{NO3}+S_{NH4}}, \frac{S_{HPO4}}{K_{HPO4,ALG}+S_{HPO4}}\right) \cdot \left(1-\frac{S_{NH4}}{K_{NH4,NO3}+S_{NH4}}\right) \cdot X_{ALG}$
2	Growth ALG NH4	$k_{gro,ALG,T0} \cdot \exp(\beta_{ALG}(T-T_0)) \cdot \frac{I(z)}{K_{I,ALG}+I(z)} \cdot \min\left(\frac{S_{NO3}+S_{NH4}}{K_{N,ALG}+S_{NO3}+S_{NH4}}, \frac{S_{HPO4}}{K_{HPO4,ALG}+S_{HPO4}}\right) \cdot \frac{S_{NH4}}{K_{NH4,NO3}+S_{NH4}} \cdot X_{ALG}$
3	Growth ZOO	$k_{gro,ZOO,T0} \cdot \exp(\beta_{ZOO}(T-T_0)) \cdot X_{ALG} \cdot \min\left(1, \frac{a_{p,ALG}}{a_{p,red}}\right) \cdot \frac{S_{O2}}{K_{O2,ZOO}+S_{O2}} X_{ZOO}$
4	Resp ALG	$k_{resp,ALG,T0} \cdot \exp(\beta_{ALG}(T-T_0)) \cdot \frac{S_{O2}}{K_{O2,resp}+S_{O2}} \cdot X_{ALG}$
5	Resp ZOO	$k_{resp,ZOO,T0} \cdot \exp(\beta_{ZOO}(T-T_0)) \cdot \frac{S_{O2}}{K_{O2,resp}+S_{O2}} \cdot X_{ZOO}$
6	Death ALG	$k_{death,ALG,T0} \cdot \exp(\beta_{ALG}(T-T_0)) \cdot X_{ALG}$
7	Death ZOO	$k_{death,ZOO,T0} \cdot \exp(\beta_{ZOO}(T-T_0)) \cdot X_{ZOO}$
8	Death ZOO Dipt	$k_{death,ZOO,Dipt,T0} \cdot \exp(\beta_{ZOO}(T-T_0)) \cdot X_{ZOO}$
9	Aer miner	$k_{miner,aero,T0} \cdot \exp(\beta_{BAC}(T-T_0)) \cdot \frac{S_{O2}}{K_{O2,miner}+S_{O2}} \cdot X_S$
10	Anox miner	$k_{miner,anox,T0} \cdot \exp(\beta_{BAC}(T-T_0)) \cdot \frac{S_{NO3}}{K_{NO3,miner}+S_{NO3}} \cdot \left(1-\frac{S_{O2}}{K_{O2,miner}+S_{O2}}\right) \cdot X_S$
11	Anae miner	$k_{miner,anae,T0} \cdot \exp(\beta_{BAC}(T-T_0)) \cdot \left(1-\frac{S_{NO3}}{K_{NO3,miner}+S_{NO3}}\right) \cdot \left(1-\frac{S_{O2}}{K_{O2,aero}+S_{O2}}\right) \cdot X_S$
12	Nitrification	$k_{nitri,T0} \cdot \exp(\beta_{BAC}(T-T_0)) \cdot \min\left(\frac{S_{O2}}{K_{O2,nitri}+S_{O2}}, \frac{S_{NH4}}{K_{NH4,nitri}+S_{NH4}}\right)$
13	P-Uptake	$k_{upt} \cdot \frac{1}{A}\left\|\frac{dA}{dz}\right\| \cdot \left(a_{P,\max}-\frac{X_{PI,S}}{X_S}\right) \cdot \frac{S_{O2}}{K_{O2,nitri}+S_{O2}} \cdot S_{HPO4} \cdot X_S$

Analysis Methodology

1. Initial simulations
2. Lake-specific calibration
3. Joint calibration for all lakes
4. Local sensitivity and dependence analysis

Iterative Process:
Repeat these steps several times

1. Initial Simulations

- Specify geometry, initial condition and input for each lake
- Simulations with prior parameter values
- Do initial sensitivity and dependence analysis
- Compare simulations with data from all lakes
- Identify and interpret major deviations

2. Lake-Specific Calibration

- Improve fit for each lake individually
- Fit a small subset of parameters
  - manually (gain understanding)
  - automatic calibration
- Find the reasons for differences in parameter estimates
- Minimize differences:
  - use non-identifiability of parameters
  - modify the model to make it more universal

3. Joint Calibration for all Lakes

- Analyse differences in estimated parameter values
- Joint calibration for all lakes
  - common values for parameter that did not differ strongly
  - different values for parameters that differed strongly
- Find reasons why these parameters have different values for different lakes

4. Local Sensitivity and Dependence Analysis

- Re-do sensitivity and dependence analysis
- Reassess:
  - the subset of fit parameters
  - the subset of parameters with different values for different lakes.
  - the degree of non-identifiability
- Return to step 2 or 3

Results

1. Initial simulations

- good results for Lake Zürich and Walensee
- poor results for Greifensee
  - Algae concentrations too low
  - Oxygen and nitrate concentrations in the hypolimnion too high

Results

2. Lake-specific calibration

- Manual calibration:
  - Improve algae simulations: increase specific death rate of zooplankton (Insect larvae)
  - Improve O_2 and NO_3 simulations: reduce thickness of the sediment layers (diffusive limitation)
- Automatic calibration of very sensitive parameters

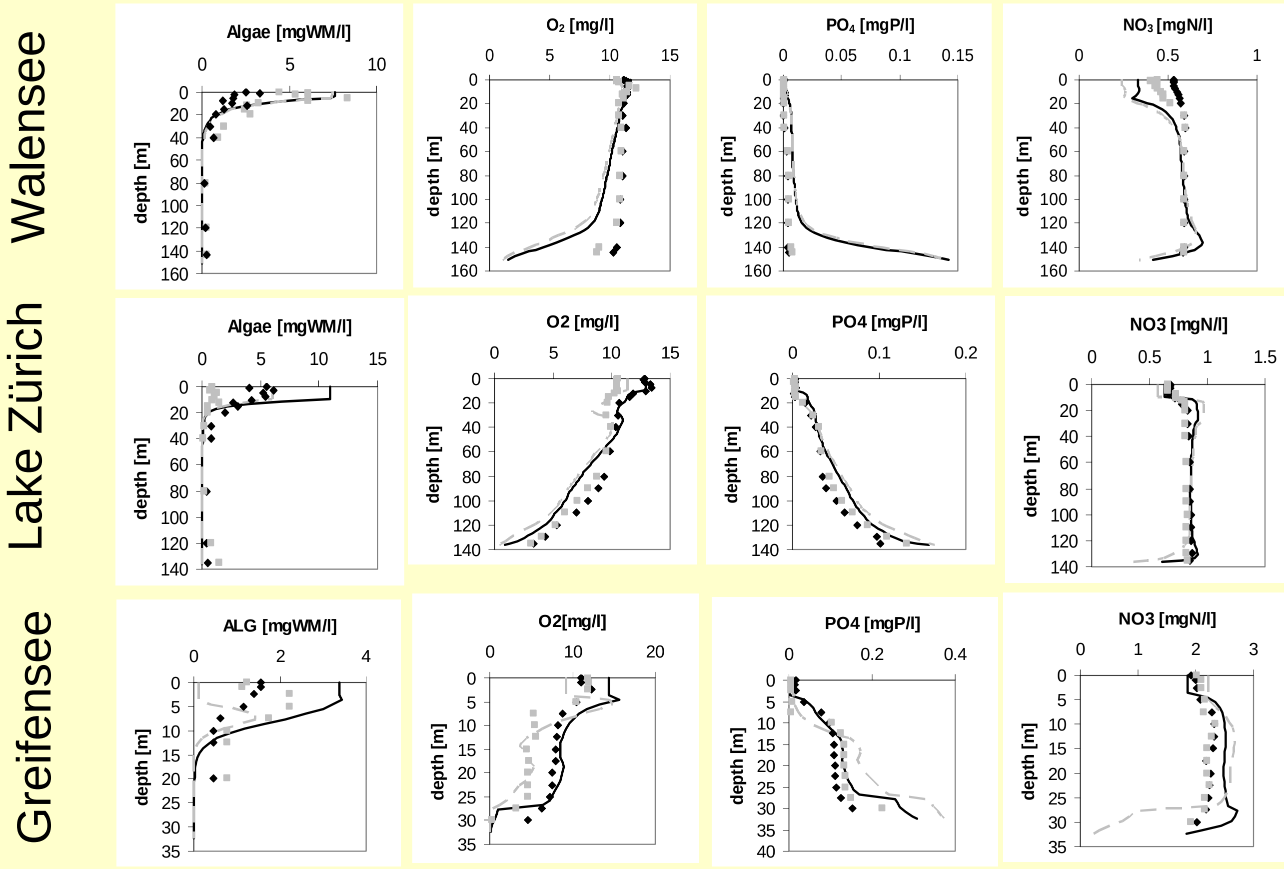
Results

3. Joint calibration for all lakes

- Only two parameters with different values for the different lakes:
  - thickness of the sediment layer
  - death rate of zooplankton
- Good overall fit

Results

3. Joint calibration for all lakes



Results

4. Local sensitivity and dependence analysis

Sensitivity ranking

Measure of global sensitivity of a parameter to model results

	All Lakes		Walensee		Zürichsee		Greifensee	
	parameter	δ_j^{msqr}	parameter	δ_j^{msqr}	parameter		parameter	δ_j^{msqr}
1	$k_{death,ZOO,T0}$	0.874	$h_{sed,1,wal}$	0.487	$k_{death,ZOO,T0}$	1.389	$k_{gro,ALG,T0}$	1.320
2	$k_{death,ALG,T0}$	0.867	$k_{death,ALG,T0}$	0.235	$k_{death,ALG,T0}$	1.315	$k_{death,ZOO,Dipt,T0}$	1.218
3	$k_{gro,ALG,T0}$	0.846	$K_{HPO4,ALG}$	0.198	$k_{resp,ALG,T0}$	0.855	$K_{I,ALG}$	0.979
4	$k_{death,ZOO,Dipt,T0}$	0.660	$k_{gro,ALG,T0}$	0.193	$k_{gro,ZOO,T0}$	0.767	$k_{resp,ALG,T0}$	0.704
5	$k_{resp,ALG,T0}$	0.654	$k_{resp,ALG,T0}$	0.180	$k_{gro,ALG,T0}$	0.718	$k_{gro,ZOO,T0}$	0.577
6	$K_{I,ALG}$	0.646	$k_{death,ZOO,T0}$	0.134	$K_{I,ALG}$	0.595	$k_{death,ALG,T0}$	0.556
7	$k_{gro,ZOO,T0}$	0.563	k_{upt}	0.119	$h_{sed,1,zue}$	0.429	$K_{HPO4,ALG}$	0.522
8	$K_{HPO4,ALG}$	0.381	$K_{I,ALG}$	0.112	$K_{HPO4,ALG}$	0.374	$k_{death,ZOO,T0}$	0.373
9	$h_{sed,1,wal}$	0.282	$k_{miner,aero,wat,T0}$	0.071	k_{upt}	0.339	$S_{HPO4,crit}$	0.298
10	$h_{sed,1,zue}$	0.262	$S_{HPO4,crit}$	0.052	$k_{resp,ZOO,T0}$	0.260	$k_{miner,anae,sed,T0}$	0.275
11	k_{upt}	0.255	$k_{miner,aero,sed,T0}$	0.037	$S_{HPO4,crit}$	0.218	$k_{miner,anox,sed,T0}$	0.266
12	$S_{HPO4,crit}$	0.211	$K_{O2,aero}$	0.032	$k_{miner,aero,sed,T0}$	0.160	k_{upt}	0.245
13	$k_{resp,ZOO,T0}$	0.161	$K_{O2,ads}$	0.031	ΔS_{HPO4}	0.092	$h_{sed,3,gre}$	0.177
14	$k_{miner,anae,sed,T0}$	0.149	ΔS_{HPO4}	0.026	$k_{miner,anox,sed,T0}$	0.060	$h_{sed,1,gre}$	0.149
15	$k_{miner,anox,sed,T0}$	0.149	$k_{resp,ZOO,T0}$	0.026	$K_{O2,aero}$	0.053	$h_{sed,2,gre}$	0.105
16	$k_{miner,aero,sed,T0}$	0.098	$k_{nitri,wat,T0}$	0.017	$K_{O2,resp}$	0.050	$K_{O2,resp}$	0.061
17	$h_{sed,3,gre}$	0.096	$K_{NH4,nitri}$	0.017	$k_{miner,aero,wat,T0}$	0.032	$K_{NO3,miner}$	0.052
18	$h_{sed,1,gre}$	0.081	$k_{gro,ZOO,T0}$	0.017	$K_{O2,ads}$	0.023	ΔS_{HPO4}	0.047
19	ΔS_{HPO4}	0.064	$K_{O2,resp}$	0.009	$k_{nitri,wat,T0}$	0.019	$k_{resp,ZOO,T0}$	0.042

1. Initial simulations
2. Lake-specific calibration
3. Joint calibration for all lakes
4. Local sensitivity and dependence analysis

Results

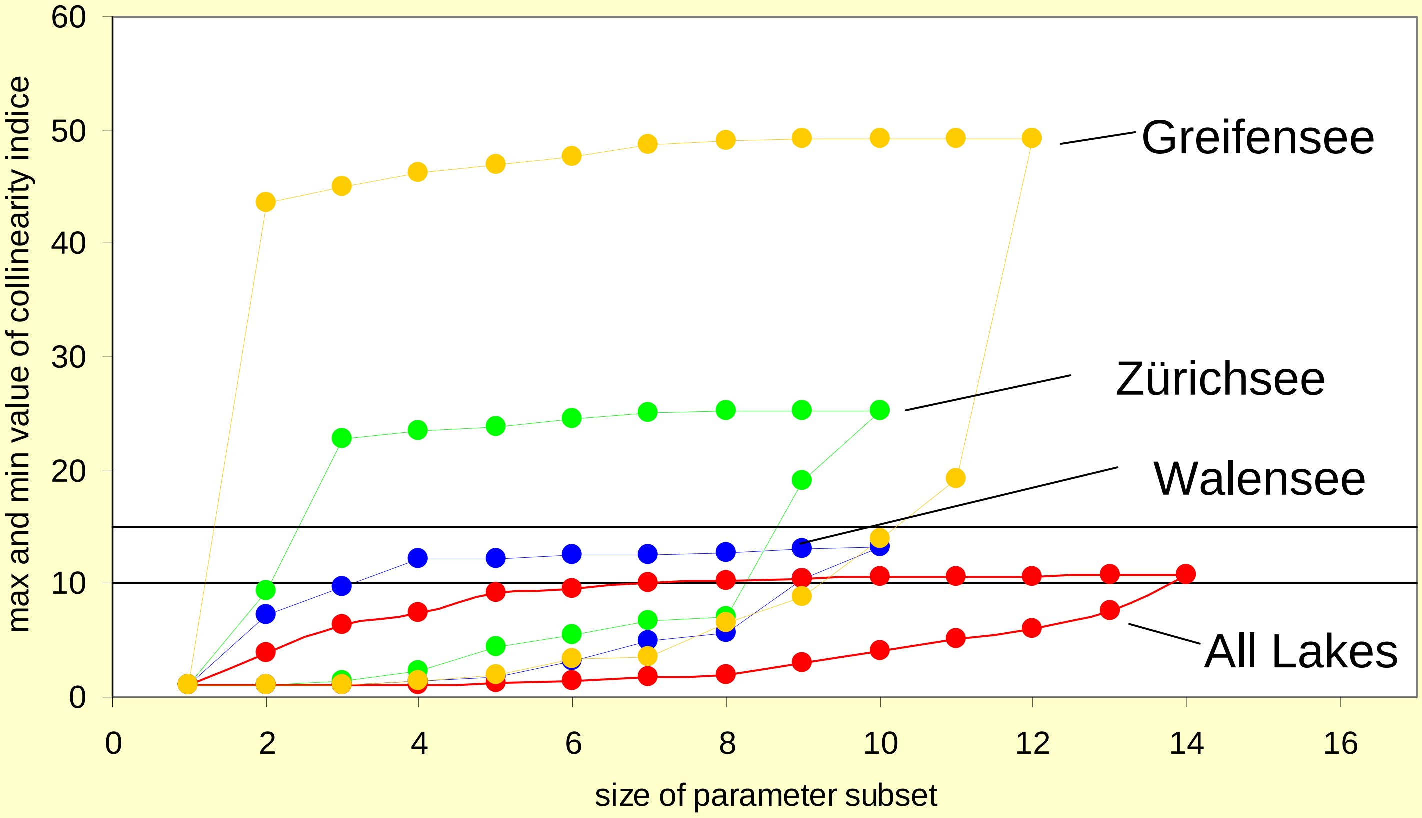
4. Local sensitivity and dependence analysis

Parameter pairs with the highest collinearity indices

	Parameter 1	Parameter2	γ
All Lakes	$k_{death,ZOO,T0}$	$k_{resp,ZOO,T0}$	12.9
	$k_{gro,ALG,T0}$	$K_{I,ALG}$	3.9
	$k_{resp,ALG,T0}$	$K_{I,ALG}$	3.5
	$k_{death,ZOO,T0}$	$k_{gro,ZOO,T0}$	2.9
	$k_{gro,ALG,T0}$	$k_{resp,ALG,T0}$	2.9
Walensee	Parameter 1	Parameter2	γ
	$k_{death,ZOO,T0}$	$k_{resp,ZOO,T0}$	14.5
	$k_{gro,ALG,T0}$	$K_{I,ALG}$	7.2
	$k_{resp,ALG,T0}$	$K_{I,ALG}$	5.8
	$K_{I,ALG}$	$K_{HPO4,ALG}$	4.9
	$k_{gro,ALG,T0}$	$K_{HPO4,ALG}$	4.5
Lake Zürich	Parameter 1	Parameter2	γ
	$k_{death,ZOO,T0}$	$k_{resp,ZOO,T0}$	40.8
	$k_{gro,ALG,T0}$	$K_{I,ALG}$	9.4
	$k_{gro,ZOO,T0}$	$k_{resp,ZOO,T0}$	7.3
	$k_{death,ZOO,T0}$	$k_{gro,ZOO,T0}$	7.1
	$k_{resp,ALG,T0}$	$K_{I,ALG}$	6.6
Greifensee	Parameter 1	Parameter2	γ
	$k_{death,ZOO,T0}$	$k_{death,ZOO,Dipt,T0}$	43.5
	$k_{resp,ALG,T0}$	$K_{I,ALG}$	6.0
	$K_{HPO4,ALG}$	$S_{HPO4,crit}$	5.2
	$k_{death,ZOO,T0}$	$k_{resp,ZOO,T0}$	5.1
	$k_{death,ZOO,Dipt,T0}$	$k_{resp,ZOO,T0}$	5.0

Results

4. Local Sensitivity and Dependence analysis



Identifiability Analysis

- Similar sensitivity ranking for all lakes
- Parameters of growth, death and respiration of algae and zooplankton have the largest influence
- The identifiability of the model parameters improves when data from all lakes are used together
- Remaining identifiability problems are avoided by adequate choice of fit parameters

Conclusions

- Good agreement of the results with data from the three lakes
- Only two parameters with lake specific values (different only in Greifensee, same in Walensee and Lake Zürich)
- Good transferability
- Reasons for differences in parameters:
  - Insect larvae
  - Simple sediment model

Outlook

- Suggestions for model improvement
  - Improve Sediment model (bacterial growth)
  - Include growth of Insect Larvae
- Improve Plankton sub-model (functional groups)
- Uncertainty analysis
- Long-term simulations (faster model)

Thank You !

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Thomas Petzoldt

Questions ?

Additional Slides

Parameter Estimation

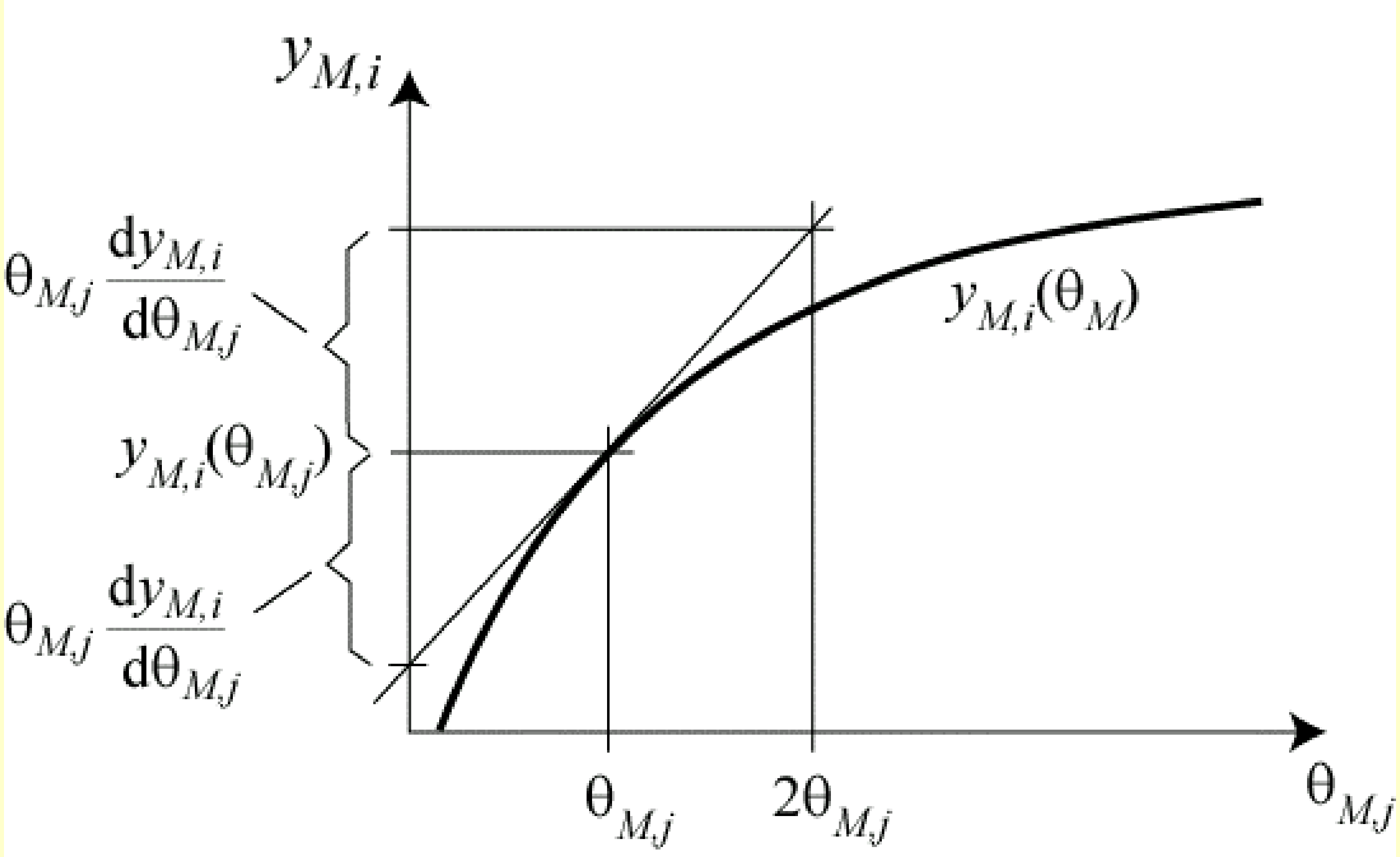
Weighted nonlinear least Squares Estimation

$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(\frac{y_{meas,i} - y_i(\boldsymbol{\theta})}{\sigma_{meas,i}} \right)^2$$

Sum of the squares of the weighted deviations of the measurement and the model results.

Local Sensitivity Analysis

- Sensitivity Functions



Local Sensitivity Analysis

- measure of global sensitivity of model results to a parameter

$$\delta_{\theta}^{msqr}(\theta) = \sqrt{\frac{1}{n}\sum_{k}\sum_{j}\sum_{i}\left(\frac{\Delta\theta_l}{sc_{yk}} \cdot \frac{\partial y_k}{\partial \theta_l}\right)^2}$$

averaging the squares of the non-dimensional error contributions for all state variables, all sampling locations and all times and taking the square root.

Dependence Analysis

- collinearity index
- the sensitivity functions are normed

$$\tilde{s}_l = \frac{s_l}{\|s_l\|}$$

- And their linear combination with minimum norm is calculated

$$\gamma(\theta) = \frac{1}{\min\limits_{\|\beta\|=1} \|\tilde{s}_1\beta_1 + \ldots + \tilde{s}_m\beta_m\|}$$

- measure of approximate linear dependence
- Serious identifiability problems start for a collinearity index between 10 and 15

Results

3. Joint Calibration for all Lakes

parameter	unit	joint fit for all lakes	Omlin *et al.* (2001a)
$K_{I,ALG}$ *	Wm^{-1}	10	34
$k_{gro,ALG,T0}$	d^{-1}	1.4	1.1
$k_{gro,ZOO,T0}$	$gDM^{-1}m^{3}d^{-1}$	0.4	0.3
$k_{death,ZOO,T0}$	d^{-1}	0.015	0.02
$k_{death,ZOO,Dipt,T0}$	d^{-1}	0.1	-
$h_{sed,1,wal}$	m	0.003	-
$h_{sed,2,wal}$	m	0.003	-
$h_{sed,1,zue}$	m	0.003	0.0036
$h_{sed,2,zue}$	m	0.003	0.0036
$h_{sed,1,gre}$	m	0.0008	-
$h_{sed,2,gre}$	m	0.0008	-
$h_{sed,3,gre}$	m	0.002	-

Results

4. Local Sensitivity and Dependence analysis

Collinearity indices

alle Seen		alle Seen		Walensee		Lake Zürich		Greifensee	
Parameter	δ_j^{msqr}	γ	γ	γ	γ	γ	γ	γ	γ
$k_{death,ZOO,T0}$	0.87	1.0		1.0		1.00		1.00	X
$k_{death,ALG,T0}$	0.87	2.8		1.0		4.3		1.18	1.00
$k_{gro,ALG,T0}$	0.85	4.4		1.8		5.9		4.7	1.9
$k_{death,ZOO,Dipt,T0}$	0.66	4.5		-		-		44.2	4.7
$k_{resp,ALG,T0}$	0.65	5.2		4.5		7.1		44.9	8.6
$K_{I,ALG}$	0.65	6.7		8.3		23.1	X	45.2	11.1
$k_{gro,ZOO,T0}$	0.56	8.7		8.4		23.6	13.2	45.4	11.1
$K_{HPO4,ALG}$	0.38	9.9		10.9	X	24.5	23.6	47.7	12.1
$h_{sed,1,wal}$	0.28	10.0		11.4	8.4	-	-	-	-
$h_{sed,1,zue}$	0.26	10.0		-	-	24.6	23.6	-	-
k_{upt}	0.26	10.0		12.6	8.4	25.2	23.7	48.4	14.3
$S_{HPO4,crit}$	0.21	10.5		13.3	10.6	25.3	25.2	48.8	18.3
$k_{resp,ZOO,T0}$	0.16	32.7	X	19.7	19.4	51.3	49.6	52.3	18.9
$k_{miner,anae,sed,T0}$	0.15	32.7	10.5	27.1	26.4	55.8	55.1	52.3	19.7
$k_{miner,anox,sed,T0}$	0.15	32.9	10.5	31.2	30.3	55.9	55.1	52.5	20.7
$k_{miner,aero,sed,T0,zue}$	0.10	33.1	10.5	-	-	56.2	55.2	-	-
$h_{sed,3,gre}$	0.10	33.9	10.5	-	-	-	-	52.9	20.7
$h_{sed,1,gre}$	0.08	34.6	10.8	-	-	-	-	53.1	20.8
ΔS_{HPO4}	0.06	35.6	11.3	35.8	34.4	58.4	57.7	55.1	21.4