Modeling in aquatic environment

Lecture 8

Water quality models

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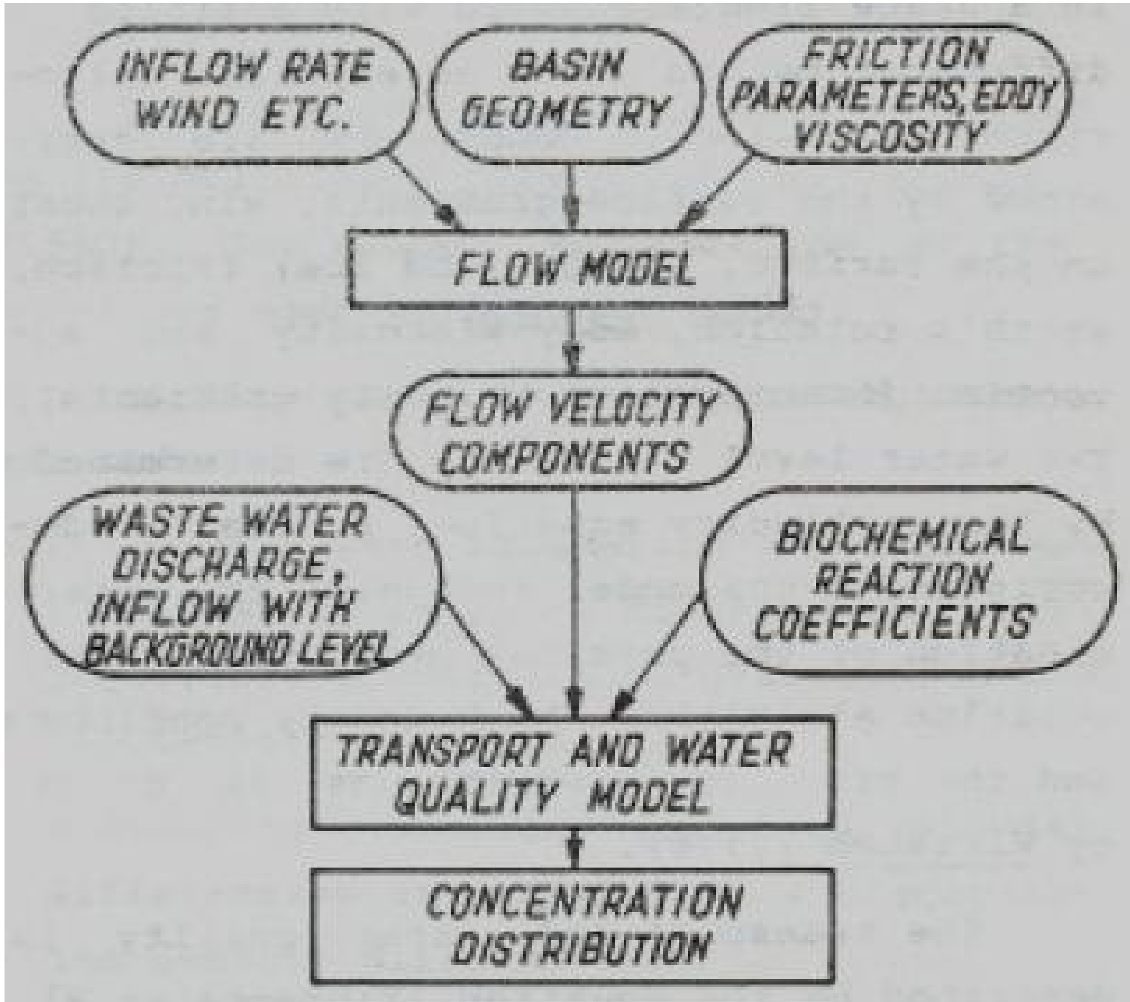


Fig. 8.

The structure of transport and water quality model

Concentration equation in general form

$$\frac{\partial c}{\partial t} = \frac{\partial qL}{\partial n} - u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - (w - w_{s1})\frac{\partial c}{\partial z}$$
$$+\frac{\partial c}{\partial x}(D_x \frac{\partial c}{\partial x}) + \frac{\partial c}{\partial y}(D_y \frac{\partial c}{\partial y}) + \frac{\partial c}{\partial z}(D_z \frac{\partial c}{\partial z})$$
$$+R(T, c...)$$

where,

- c = concentration of simulated substance, qL= amount of loading release , n= length measure against release, u,v,w = advective velocity components in x-, y- ja z- directions, w_{s1} or w_s = settling velocity in the case of suspended solids, for soluble substances some value of w_{s1} is calibrated (!) , D_x, D_y, D_z = dispersion coefficients, R(T,c) = biogeochemical changes in substance concentration

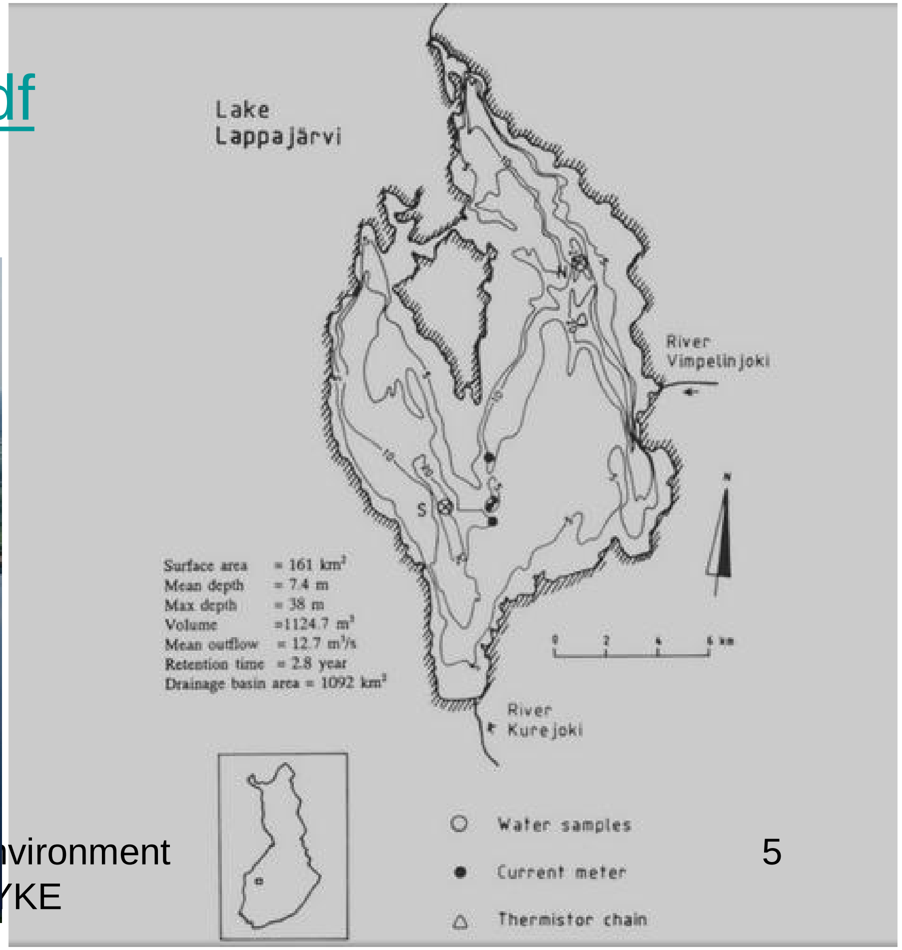
Application of WQ-models

- We include :
  - Advection
  - Dispersion
  - Settling in water column and deposition on the bottom
- Bio- chemical processes
  - Decomposition, respiration, aeration, anaerobic release of P from the bottom
  - Select the most important variables concerning the problem
  - Oxygen, nutrients (like P,N), chlorophyll-a and some conservative substance (like Na)
  - Limiting factors (light, nutrients, …) must be included
  - Temperature corrections must be included

Lake Lappajärvi WQ-model

(Malve et al. 1991)

- PROBE temperature model
  - Materials\Effects of Climate Change....pdf
- PROBE-WQ model
  - Materials\Lappajarvi_WQ.pdf



Oxygen model

Computation of dissolved oxygen Both abiotic and biotic factors affect the concentration of oxygen. The change of dissolved oxygen concentration as a function of time is described by the following equation':

$$\frac{dO_2}{dt} = K' \times \sqrt{W} \times (O_{2sat} - O_2) - K_1 \times BOD_7 \times BRAT + \mu \times \alpha_1 \times CH - r \times \alpha_2 \times CH - \frac{SOD \times AREA}{V} \quad (7)$$

K' = aeration constant = 2.0 • 10^{-4} cm/d, W = wind speed, z = layer thickness
O_{2sat} = dissolved oxygen saturation concentration at the surface layer temperature
O_2 = dissolved oxygen concentration at the surface layer temperature
K_1 = BOD decay rate = 0.1 l/d (function of temperature, f(T))
BOD, = BOD_7 concentration
BRAT = BOD/BOD_7 = 1.5
α_1, α_2 = stoichiometric coefficients for growth and respiration= 0.1903
μ = growth rate of algae
r = algal respiration coefficient = 0.065 1/d, (f(T))
CH = chlorophyll concentration
SOD = bottom sediment oxygen demand, (f(T))
AREA = area of the bottom sediment
V = volume of the water body

The first term on the right hand side describes aeration in the surface layer, the second one biological oxygen demand, the third and fourth ones phytoplankton growth and respiration, and the last one bottom sediment oxygen demand.

Phytoplankton biomass and ToTP

Computation of phytoplankton biomass Chlorophyll-a concentration is used as a relative measure of phytoplankton biomass. The rate of change of phytoplankton biomass is expressed as [8]

$$\frac{dCH}{dt} = \mu \times CH - r \times CH - \frac{SED}{h} \times CH \qquad (8)$$

Phosphorus cycle Description of the phosphorus cycle is quite simple. Total phosphorus concentration in the lake is affected by external loading, phosphorus sedimentation and release of phosphorus under unaerobic conditions.
The change of total phosphorus concentration as a function of time is described by the following equation [8]

$$\frac{dTOTP}{dt} = -\frac{SEDP}{h} \times (TOTP)^2 + LOAD + \frac{RELEASE}{AREA \times h} \qquad (11)$$

SEDP = net phosphorus sedimentation coeffkient = 0.002 (m/d)/(µg/l) .
LOAD = external loading
RELEASE = rate of phosphorus release from the sediment under anaerobic conditions

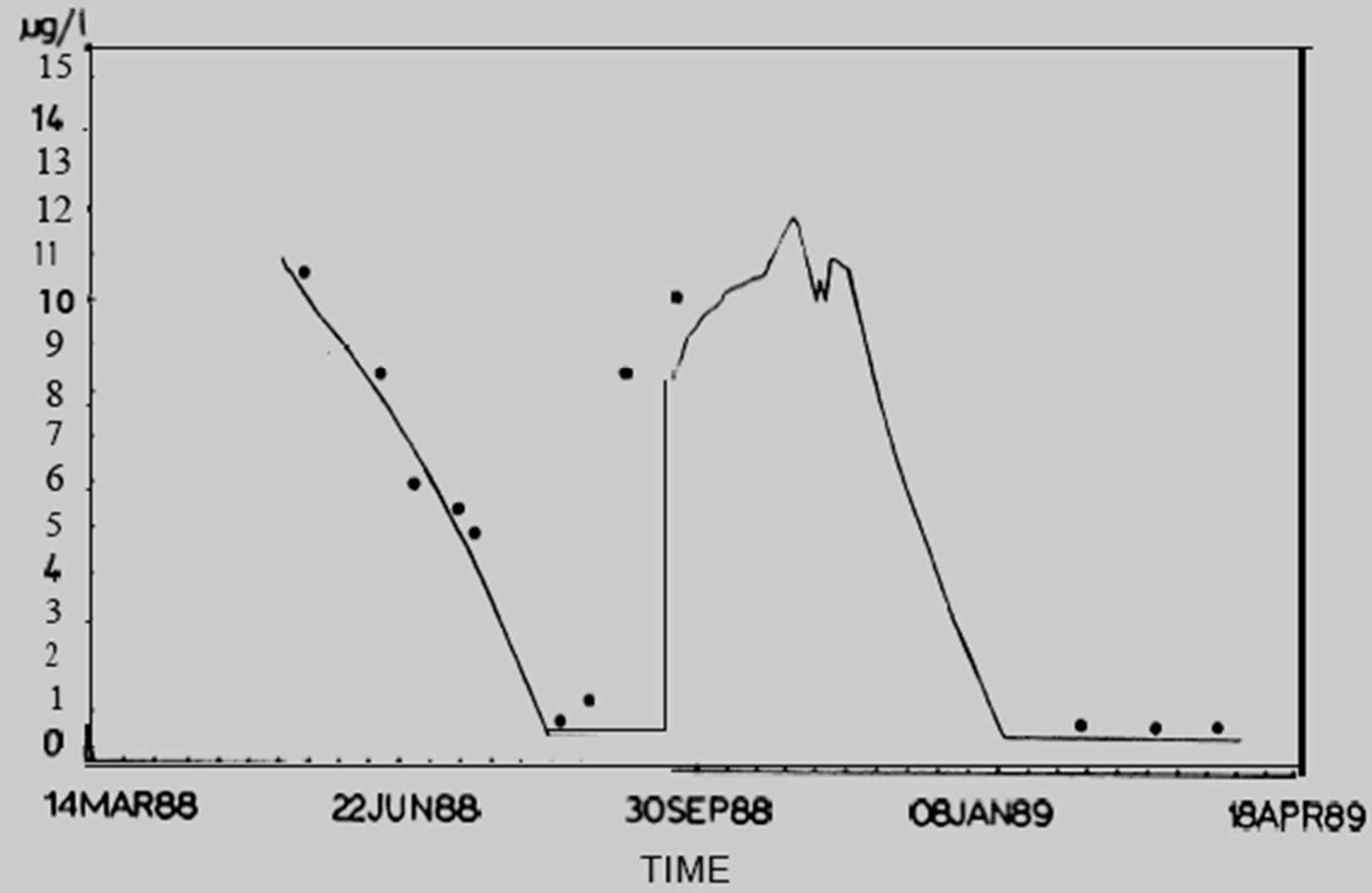


Figure 7. Observed (.) and calculated (–) oxygen concentrations in bottom layer (height 1 m). Calibration, summer 1988.

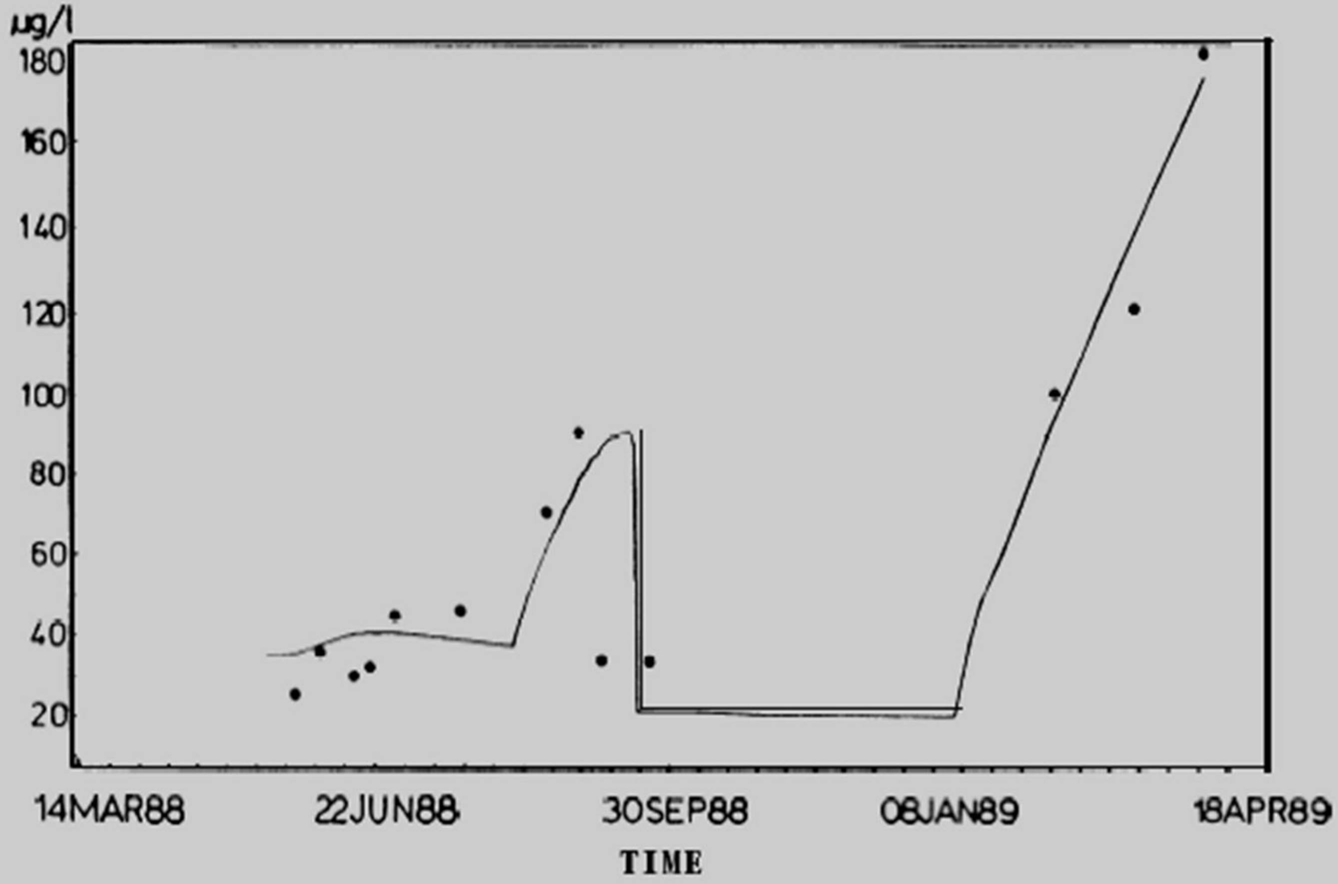


Figure 8. Observed (.) and calculated (–) total phosphorus concentrations in bottom layer (height 1 m). Calibration, summer 1988.

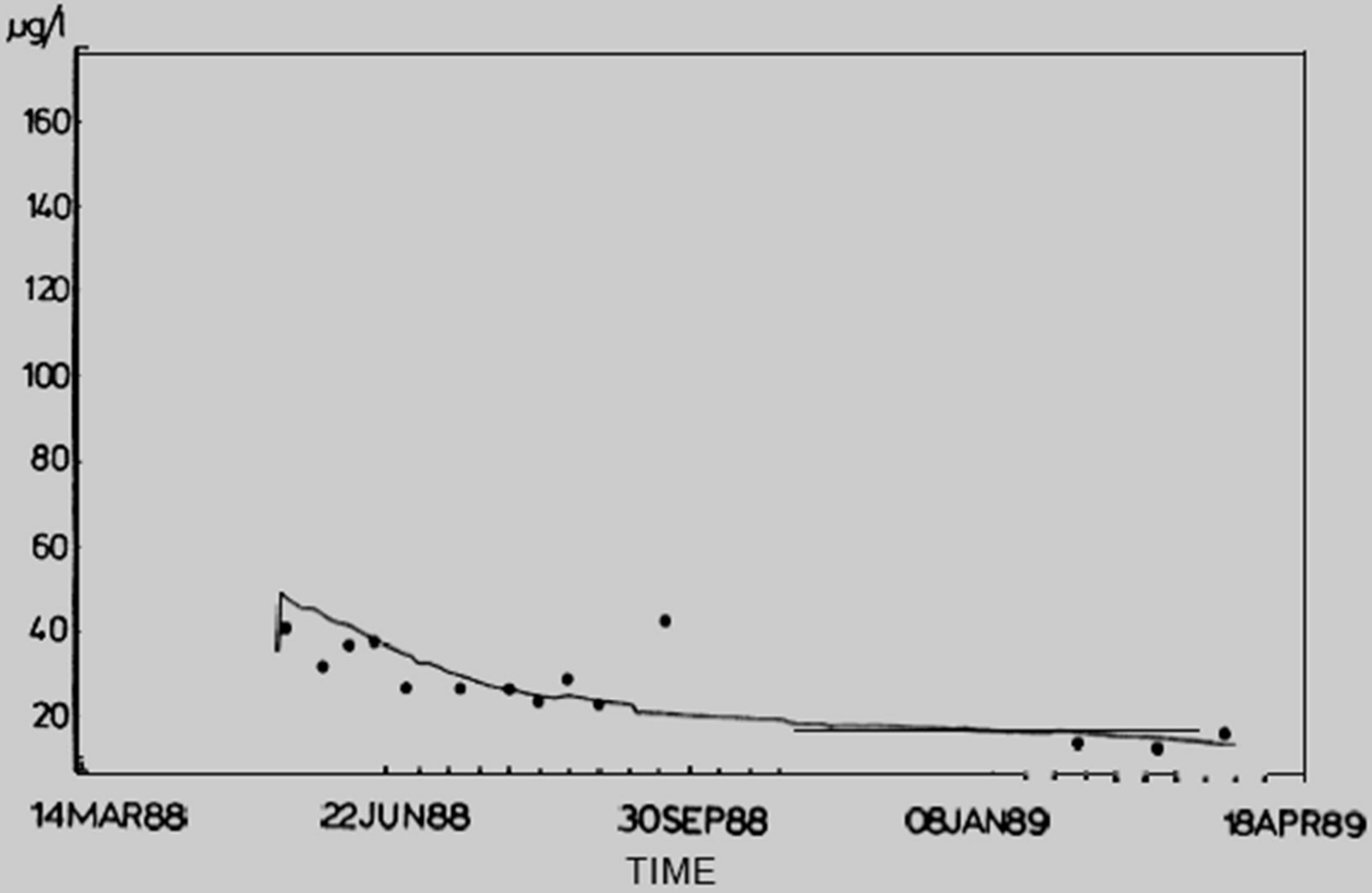


Figure 9. Observed (.) and calculated (–) total phosphorus concentrations in surface (O-l m) layer. Calibration, summer 1988.

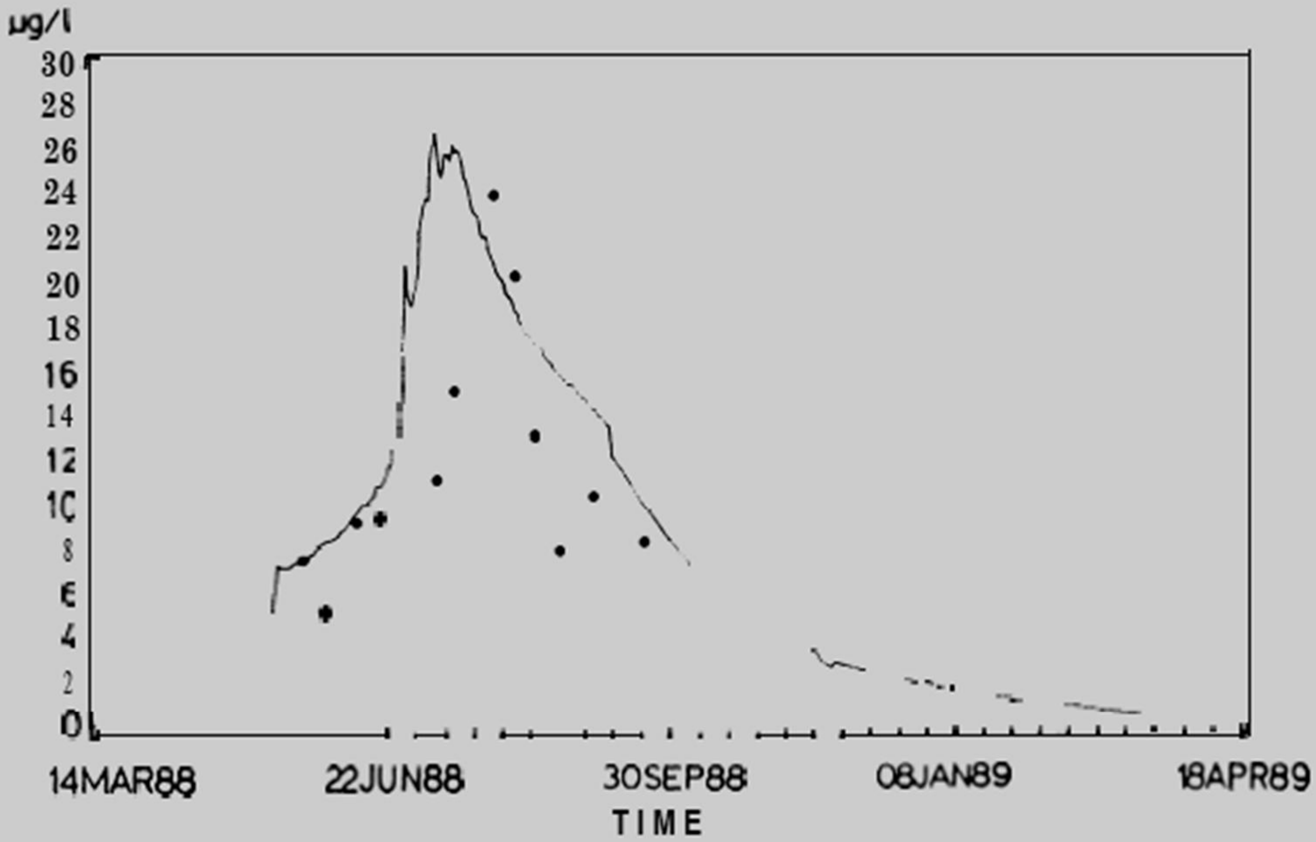


Figure 10. Observed (.) and calculated (-) chlorophyll-a concentrations in surface (O-1 m) layer. Calibration, summer 1988.

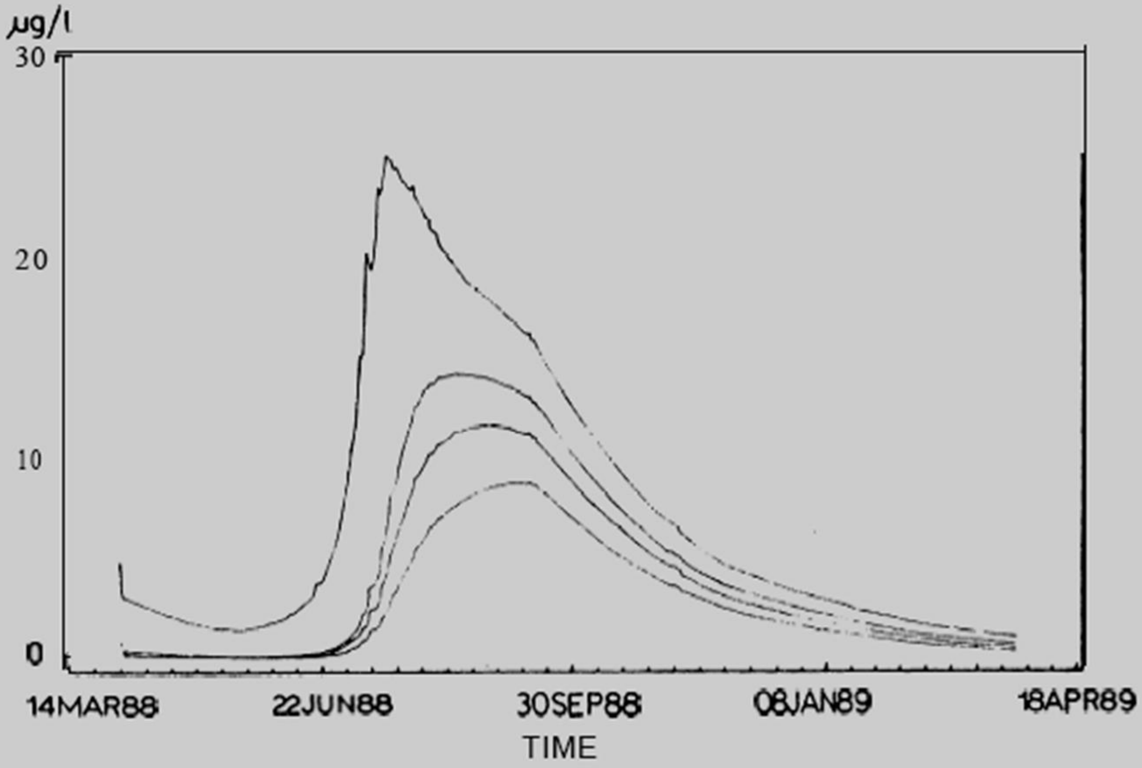


Fig. 11 Calculated chlorophyll-a concentration with loading levels 1 - 4.

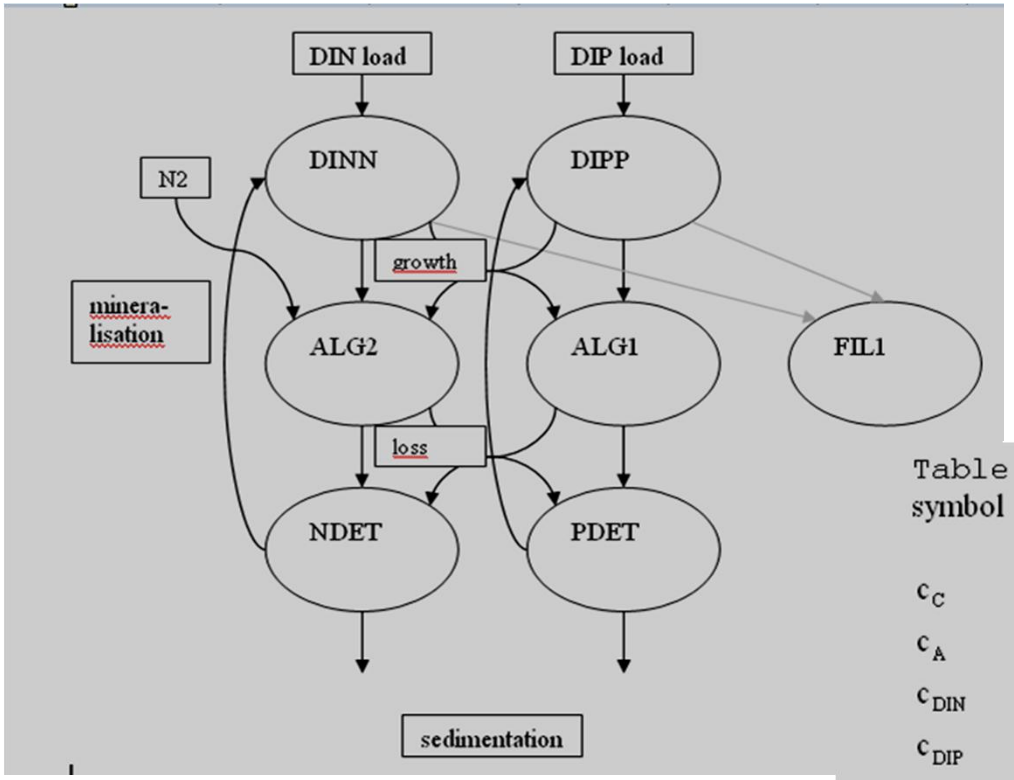
1. Present total phosphorus loading 55 697 kg/year

2. Fast obtainable loading level 47 469 kg/year
-reduction of the present loading 14.8%

3. Desirable loading level 37 483 kg/year
-reduction of the present loading 32.7%

4. Loading level with the best available protection measures 30 689 kg/year
-reduction of the present loading 44.9%

Interactions in EIA-SYKE-model



- DIP=dissolved inorganic P
- DIN=dissolved inorganic N
- Detritus= ‘dead’ particulate organic material in water

Table 1. Model variables.

symbol	definition	unit
c_C	Biomass of cyanobacteria (wet weight)	g m^{-2}
c_A	Biomass of the other algae (wet weight)	g m^{-2}
c_{DIN}	DIN concentration	mg m^{-3}
c_{DIP}	DIP concentration	mg m^{-3}
c_{Ndet}	Detritus nitrogen	mg m^{-3}
c_{Pdet}	Detritus phosphorus	mg m^{-3}
L_{DIN}	DIN load	mg m^{-3} d^{-1}
L_{DIP}	DIP load	mg m^{-3} d^{-1}
I	Total radiation	MJ m^{-2}d^{-1}
T	Temperature	^{o} C
Ice	Ice-cover (0,1)	-
t	Time	d
h	Depth of grid cell	m

Table 2. Model parameters

Symbol	definition	reference	value	unit
N_{inC}	Nitrogen in cyanobacteria	Redfield, 1958	0.0193	-
P_{inC}	Phosphorus in cyanobacteria	Redfield, 1958	0.00268	-
N_{inA}	Nitrogen in the other algae	Redfield, 1958	0.0193	-
P_{inA}	Phosphorus in the other algae	Redfield, 1958	0.00268	-
μ_{Cmax}	Maximal growth rate of cyanobacteria	calibration	0.5	d^{-1}
μ_{Amax}	Maximal growth rate of the other algae	Olli *et al.*, 1996	0.7	d^{-1}
R_{Cmax}	Maximum loss rate of cyanobacteria	calibration	0.1	d^{-1}
R_{Amax}	Maximum loss rate of the other algae	calibration	0.15	d^{-1}
K_{NC}	Half-saturation coefficient of DIN for cyanobacteria	Tyrrell, 1999	0	$mg\ m^{-3}$
K_{PC}	Half-saturation coefficient of DIP for cyanobacteria	Kononen & Leppänen, 1997	2	$mg\ m^{-3}$
K_{NA}	Half-saturation coefficient of DIN for the other algae	calibration	7	$mg\ m^{-3}$
K_{PA}	Half-saturation coefficient of DIP for the other algae	calibration	1	$mg\ m^{-3}$
K_{IC}	Half saturation coefficient of radiation for cyanobacteria	calibration	20	$MJ\ m^{-2}\ d^{-1}$
K_{IA}	Half saturation coefficient of radiation for the other algae	calibration	15	$MJ\ m^{-2}\ d^{-1}$
C_{min}	Minimum biomass of cyanobacteria	calibration	0.5	$g\ m^{-2}$
A_{min}	Minimum biomass of the other algae	calibration	0.01	$g\ m^{-2}$
A_{max}	Maximum total biomass of algae	calibration	300	$g\ m^{-2}$
β_0	Maximal detritus nitrogen mineralisation rate	Garber, 1984	0.018	d^{-1}
γ_0	Maximal detritus phosphorus mineralisation rate	Garber, 1984	0.043	d^{-1}
ν_{Ndet}	Settling rate of detritus nitrogen	Heiskanen & Tallberg, 1999	1	$m\ d^{-1}$

ν_{Ndet}	Settling rate of detritus nitrogen	Heiskanen & Tallberg, 1999	1	m d^{-1}
ν_{Pdet}	Settling rate of detritus phosphorus	Heiskanen & Tallberg, 1999	1	m d^{-1}
S_{Ndet}	Sedimentation rate of detritus nitrogen	calibration	0.16	m d^{-1}
S_{Pdet}	Sedimentation rate of detritus phosphorus	Lehtoranta, 1998	0.00	m d^{-1}
T_{opt}	Optimal temperature			
	for the growth of cyanobacteria	Kononen & Leppänen, 1997	25	°C
	for the growth of the other algae	calibration	15	°C
	for losses	calibration	25	°C
	for detritus nitrogen mineralisation	Garber, 1984	18	°C
	for detritus phosphorus mineralisation	Garber, 1984	18	°C
a_T	Coefficient for temperature limiting factor			
	for the growth of cyanobacteria	calibration	1.14	-
	for the growth of the other algae	calibration	1.001	-
	for losses	calibration	1.05	-
	for detritus nitrogen mineralisation	Garber, 1984	1.31	-
	for detritus phosphorus mineralisation	Garber, 1984	1.60	-
I_{red}	Radiation attenuation by ice	calibration	0.5	-
h_{mix}	Depth of mixing layer	calibration	20	m

Table 3. Model equations, rates and limiting factors.

Equations

$$\frac{\partial c_C}{\partial t} = (\mu_C - R_C) c_C \qquad (1)$$

$$\frac{\partial c_A}{\partial t} = (\mu_A - R_A) c_A \qquad (2)$$

$$\frac{\partial c_{DIN}}{\partial t} = \beta\, c_{NDet} - \mu_A N_{inA} c_A h_{mix}^{-1} - \mu_C N_{inC} c_C h_{mix}^{-1} + L_{DIN} \qquad (3)$$

$$\frac{\partial c_{DIP}}{\partial t} = \gamma\, c_{Pdet} - \mu_A P_{inA} c_A h_{mix}^{-1} - \mu_C P_{inC} c_C h_{mix}^{-1} + L_{DIP} \qquad (4)$$

$$\frac{\partial c_{Ndet}}{\partial t} = N_{inA}\ R_A c_A h_{mix}^{-1} + N_{inC}\ R_C c_C h_{mix}^{-1} - \beta c_{Ndet} - \nu_{Ndet} c_{Ndet} h^{-1} - S_{Ndet} c_{Ndet} h^{-1} \qquad (5)$$

$$\frac{\partial c_{Pdet}}{\partial t} = P_{inA}\ R_A c_A h_{mix}^{-1} + P_{inC}\ R_C c_C h_{mix}^{-1} - \gamma c_{Pdet} - \nu_{Pdet} c_{Pdet} h^{-1} - S_{Pdet} c_{Pdet} h^{-1} \qquad (6)$$

Rates

$$\mu_C = \mu_{Cmax} f_{CN}(c_{DIN}, c_{DIP})\ f_{CI}(I)\ f(T) f_{AC}(c_A, c_C) \qquad (7)$$

$$\mu_A = \mu_{Amax} f_{AN}(c_{DIN}, c_{DIP})\ f_{AI}(I)\ f(T) f_{AC}(c_A, c_C) \qquad (8)$$

$$R_C = R_{Cmax} f(T)(c_C - C_{min})/c_C \qquad (9)$$

$$R_A = R_{Amax} f(T)(c_A - A_{min})/c_A \qquad (10)$$

$$\beta = \beta_0 f(T) \qquad (11)$$

$$\gamma = \gamma_0 f(T) \qquad (12)$$

Institute, SYKE

Limiting factors

$$f_{CN}(c_{DIN}, c_{DIP}) = \frac{c_{DIN}}{c_{DIN} + K_{NC}} \frac{c_{DIP}}{c_{DIP} + K_{PC}} \quad (13)$$

$$f_{AN}(c_{DIN}, c_{DIP}) = \frac{c_{DIN}}{c_{DIN} + K_{NA}} \frac{c_{DIP}}{c_{DIP} + K_{PA}} \quad (14)$$

$$f\ (T) = \exp\left[\int_{T_{opt}}^{T} \ln \theta dT\right], \text{ where } \theta = a_T + (1 - a_T) T / T_{opt} \quad (15)$$

$$f_{CI}(I) = \frac{I(1 - IceI_{red})}{I(1 - IceI_{red}) + K_{IC}} \quad (16)$$

$$f_{AI}(I) = \frac{I(1 - IceI_{red})}{I(1 - IceI_{red}) + K_{IA}} \quad (17)$$

$$f_{AC}(c_A, c_C) = 1 - \frac{c_A + c_C}{A_{max}} \quad (18)$$

Summary of WQ-model calculations

- Check that you have data to describe WQ in variable discharge and loading conditions
- Select those properties (variables), which describe best the effects of loading and concentrate calibration on them
- Use most simple parameterization of the variables
- First coefficient values from literature and by experience
- Compare the calculated and observed values of the selected variables
- Calibrate model tuning parameter values
- Select the conditions/scenarios (weather, discharge and loading) during which the effects are described ….and run the model!!