Advanced Environmental Systems Analysis [mod.1]

AESA – A. Y. 2023/24 – 1st semester

4th practice – Lake2K

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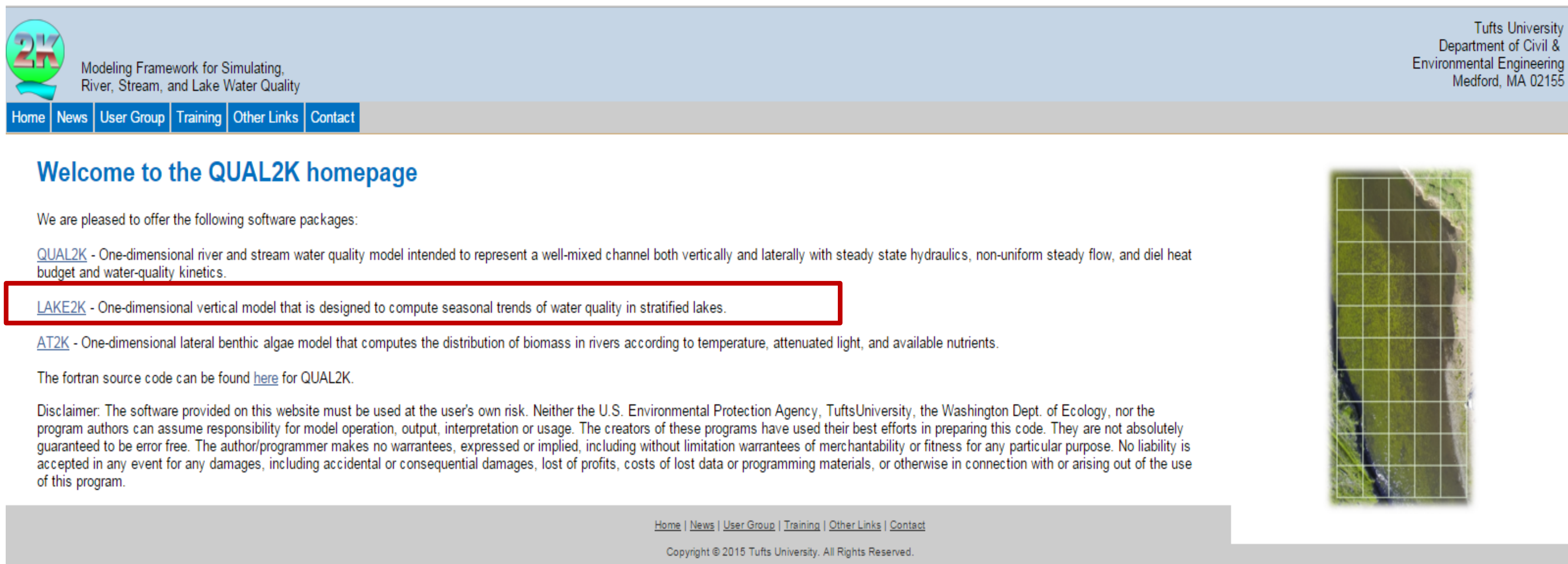
Lake2k

- One-dimensional vertical model that is designed to compute seasonal trends of water quality in stratified lakes.
- http://qual2k.com/


Modeling Framework for Simulating, River, Stream, and Lake Water Quality

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Welcome to the QUAL2K homepage

We are pleased to offer the following software packages:

QUAL2K - One-dimensional river and stream water quality model intended to represent a well-mixed channel both vertically and laterally with steady state hydraulics, non-uniform steady flow, and diel heat budget and water-quality kinetics.

LAKE2K - One-dimensional vertical model that is designed to compute seasonal trends of water quality in stratified lakes.

AT2K - One-dimensional lateral benthic algae model that computes the distribution of biomass in rivers according to temperature, attenuated light, and available nutrients.

The fortran source code can be found here for QUAL2K.

Disclaimer: The software provided on this website must be used at the user's own risk. Neither the U.S. Environmental Protection Agency, TuftsUniversity, the Washington Dept. of Ecology, nor the program authors can assume responsibility for model operation, output, interpretation or usage. The creators of these programs have used their best efforts in preparing this code. They are not absolutely guaranteed to be error free. The author/programmer makes no warranties, expressed or implied, including without limitation warrantees of merchantability or fitness for any particular purpose. No liability is accepted in any event for any damages, including accidental or consequential damages, lost of profits, costs of lost data or programming materials, or otherwise in connection with or arising out of the use of this program.

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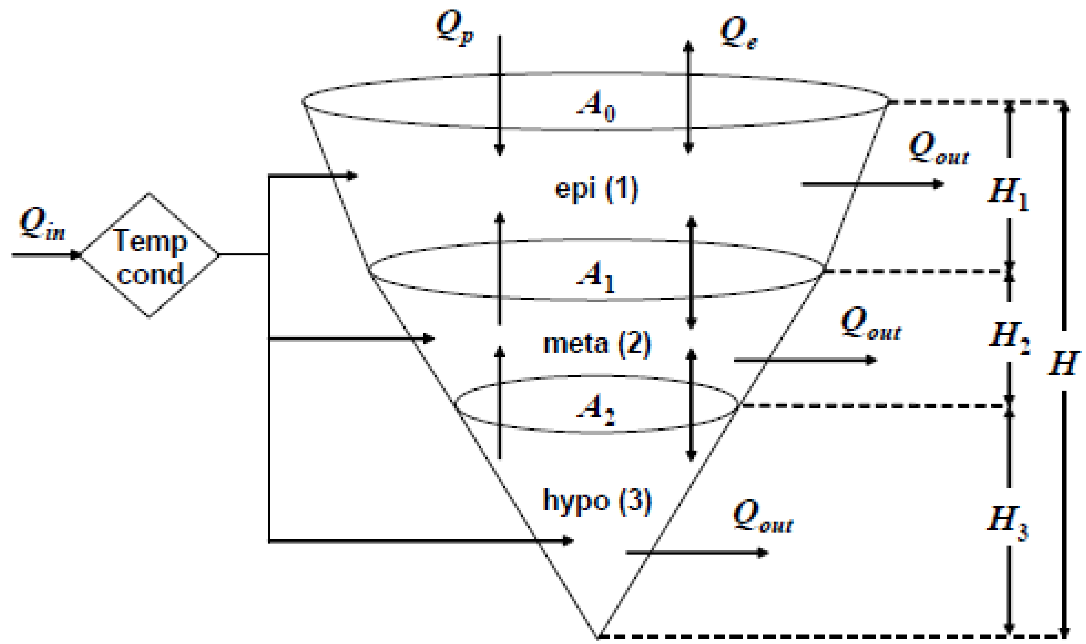
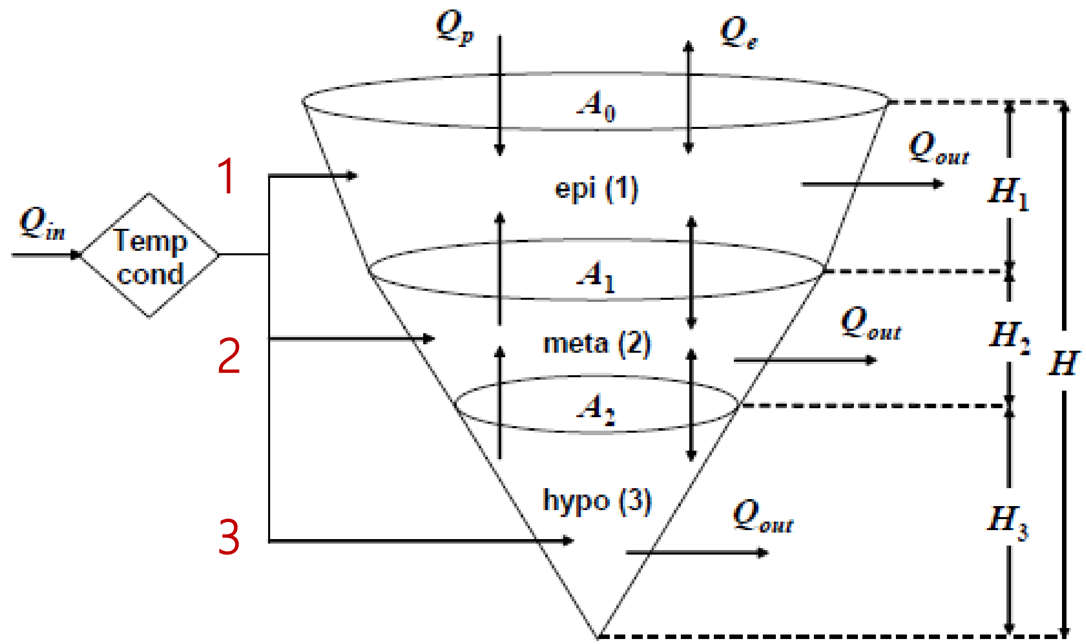
- Click on the link LAKE2K to download the zip-folder

Model - Physics



The model presently simulates the lake as a one-dimensional system consisting of **three vertical layers**.
The volumes of the two deeper layers (**metalimnion** and **hypolimnion**) are held fixed whereas the **epilimnion** is allowed to change as a function of the balance between inflows and outflows.

Model - Physics



The inflow is routed into one of the layers depending on the density of the inflow and the layer according to the algorithm:

1. If the inflow density is less than the average of the epilimnion and metalimnion densities, the inflow enters the epilimnion.
2. If the inflow density is greater than the average of the metalimnion and hypolimnion densities, the inflow enters the hypolimnion.
3. Otherwise, the inflow enters the metalimnion.

Model – Water balance

A dynamic water balance is computed for the lake as in

$$\frac{dV}{dt} = Q_{in} + Q_p - Q_e - Q_{out}$$

where
V = lake volume [m3]
t = time (d)
Qin = inflow [m3/d]
Qp = precipitation flow [m3/d]
Qe = evaporation flow [m3/d]
Qout = outflow [m3/d]

This equation is integrated to simulate how the lake's volume changes as a function of time.

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Qout = outflow [m3/d]

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Model – Water balance

Evaporation flow

The model internally computes the loss of water due to evaporation. This flow is computed as

$$Q_e = \frac{J_e A_0}{\rho L_e} \times \frac{\text{m}}{100\ \text{cm}}$$

where *Je = the heat flux due to evaporation [cal/cm²/d]*

ρ = the density of water [=1 g/cm³],

Le = the latent heat of vaporization [cal/g].

The latent heat is related to temperature by

$$L_e = 597.3 - 0.57 T_1$$

where *T1 = the temperature of the epilimnion [°C].*

The heat flux due to evaporation is computed as a function of wind speed, the dew-point temperature and the epilimnion temperature.

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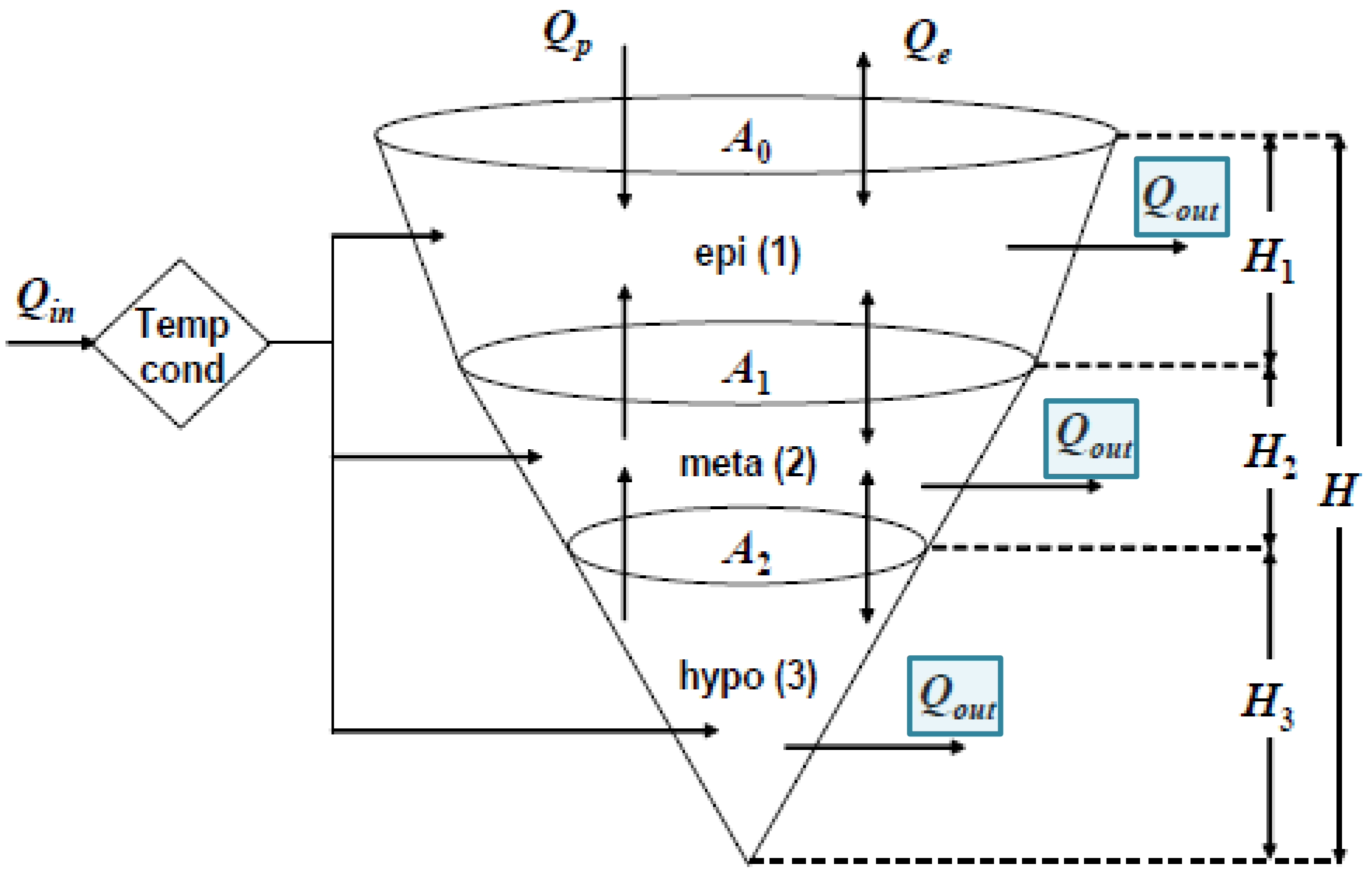
This equation is integrated to simulate how the lake's volume changes as a function of time.

Model – Water balance

Outflow



Model – Water balance

Outflow

single out-flow position

Seven options are available to compute outflow. The desired method is chosen using the pull-down menu in cell B6 on the **Outflow worksheet**.

$Q_{out}=Q_{in}$

- Flowout(epi)=Flowin. The outflow is set equal to the inflow and exits the lake from the epilimnion. Note that if the Outflow Mode is left blank, this is the default option.
- Flowout(meta)=Flowin. The outflow is set equal to the inflow, and exits the lake from the metalimnion.
- Flowout(hypo)=Flowin. The outflow is set equal to the inflow, and exits the lake from the hypolimnion.

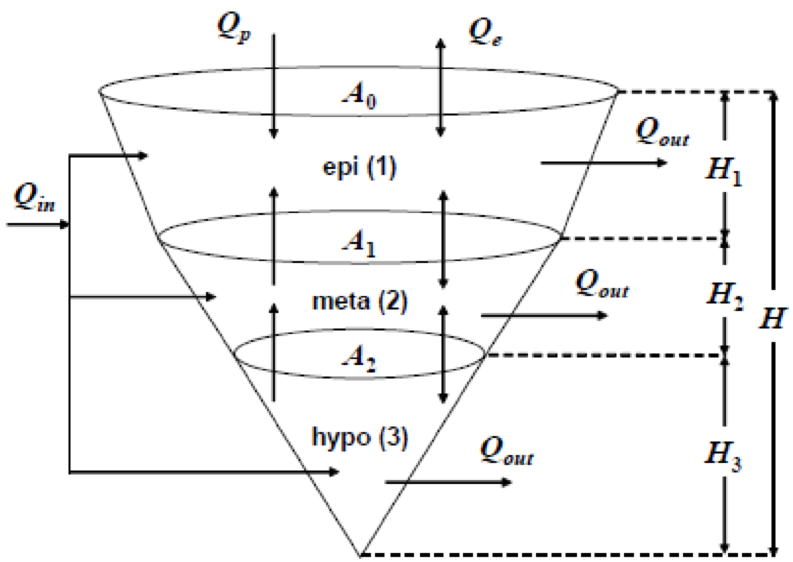
The user can enter a time series of outflows into columns A and B. The program uses linear interpolation to determine values between the entered dates.

- Time Series (epi): the outflow exits the lake from the epilimnion.
- Time Series (meta): the outflow exits the lake from the metalimnion.
- Time Series (hypo): the outflow exits the lake from the hypolimnion.

Time-series

- Stage-Discharge. The user can enter a stage-discharge curve in tabular form in columns D and E. The program uses linear interpolation to determine intermediate values.

Model – Vertical segmentation and mixing



The metalimnion and hypolimnion are set at fixed volumes whereas the epilimnion volume is allowed to vary.

The inflow is entered into one of the layers depending on the inflow's density as well as the density of the layers.

If necessary (that is, if the flow enters the hypolimnion or metalimnion), the flow is routed through the other layers and exits through either the epilimnion or the hypolimnion depending on the user's choice of outflow mode.

The density is related to water temperature and dissolved solids.

Model – Vertical segmentation and mixing

The model uses turbulent diffusion to mix water between the layers.
For example, for a **conservative substance** with no flow, a mass balance for the metalimnion can be written as

$$\frac{dc_2}{dt} = \frac{E_1'}{V_2}(c_1 - c_2) + \frac{E_2'}{V_2}(c_3 - c_2)$$

where
c_i = the concentration in layer i [g/m^3]
i = 1, 2, and 3 for the epi-, meta- and hypolimnion, respectively,
V_i = the volume of layer i [m^3]
E_i' = the bulk turbulent diffusion coefficient across the lower boundary of layer i [m^3/d]
it is related to more fundamental quantities by

$$E_i' = \frac{E_i A_i}{(H_i + H_{i+1})/2}$$

where
E_i = the turbulent diffusion coefficient across the lower boundary of layer i [m^2/d]
A_i = the surface area of the lower boundary of layer i [m^2]
H_i = the thickness of layer i [m]

Model – Vertical segmentation and mixing

Two options (Mixing modes) are available to determine the turbulent diffusion coefficients using the pull-down menu in cell b6 of the Vertical Mixing Worksheet.

These are:

1. Munk-Anderson (page 31 of pdf* document)
This approach employs a model to compute vertical mixing between layers based on **wind speed and water density** developed originally by Munk and Anderson (1948).

2. Time series:
Vertical turbulent diffusion coefficients between the layers can be entered as a time series.
The program uses linear interpolation to determine the mixing coefficients between the entered dates.

	A	B	C
1	LAKE2K		
2	Lake Water Quality Model		
3	Lake Washington		
4	Vertical Mixing		
5			
6	Mixing mode	Munk-Anderson	
7	a coefficient	20.00	
8	c coefficient	5.00	
9			
10	Time Series:	Vertical Diffusion	Vertical Diffusion
11		Epi-Meta	Meta-Hypo
12	Time (d)	cm2/s	cm2/s
13	1/1/00	5.00	5.00
14	1/17/00	0.01	0.01
15	2/19/00	0.01	0.01
16	2/20/00	5.00	5.00
17	3/7/00	5.00	5.00
18	3/23/00	5.00	5.00
19	4/1/00	0.04	0.04
20	5/30/00	0.04	0.01
21	9/15/00	0.04	0.01
22	10/1/00	1.00	0.02
23	11/1/00	5.00	5.00
24	1/1/01	5.00	5.00

*L2KDocVersion1_04_20_June_2012.pdf

Model – Temperature model

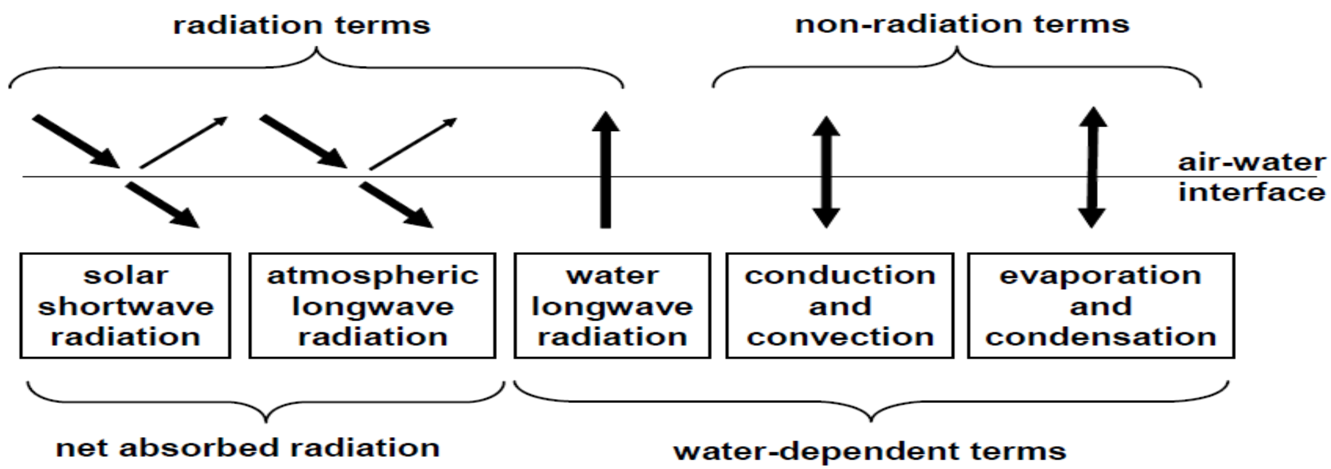
A heat balance is written for each vertical layer (epilimnium, metalimnium, hypolimnium).

The lake temperature profile is influenced by different phenomena

1. Surface heat flux → epilimnion

It is modeled as a combination of 5 processes (shortwave solar radiation, longwave atmosferic radiation, water longwave radiation, conduction and convection, condensartion and evaporation).

This balance depends on meteorological variables (air temperature, wind etc.), but also on lake conditions (e.g., water temperature)



2. Ice model

Model – Constituents

Model – Constituents

Model kinetics and mass transfer processes.

The state variables are:

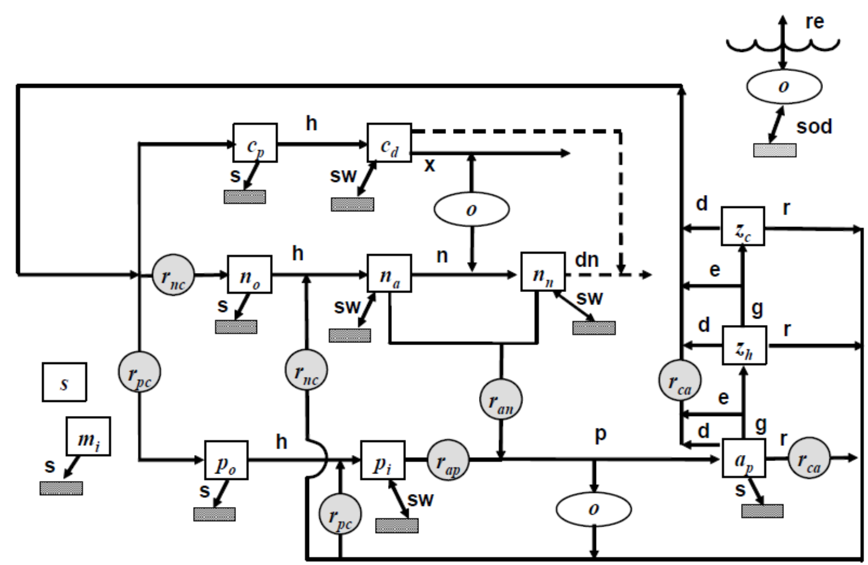
	Variable	Symbol	Units*
	Conductivity	s	μmhos
	Inorganic suspended solids	m_i	mgD/L
	Dissolved oxygen	o	mgO_2/L
C	Particulate organic carbon	c_p	mgC/L
C	Dissolved organic carbon	c_f	mgC/L
N	Organic nitrogen	n_o	μgN/L
N	Ammonia nitrogen	n_a	μgN/L
N	Nitrate nitrogen	n_n	μgN/L
P	Organic phosphorus	p_o	μgP/L
P	Inorganic phosphorus	p_i	μgP/L
	Organic silica	s_o	mgSi/L
	Inorganic silica	s_i	mgSi/L
	Phytoplankton	a_{p1}	μgA/L
	Herbivorous zooplankton	z_h	mgC/L
	Carnivorous zooplankton	z_c	mgC/L
	Phytoplankton2	a_{p2}	μgA/L
	Phytoplankton3	a_{p3}	μgA/L

* $mg/L \equiv g/m^3$ and $\mu g/L \equiv mg/m^3$

Model – Constituents

Kinetic processes are
hydrolysis (h)
oxidation (x)
nitrification (n) and denitrification (dn)
photosynthesis (p) and respiration (r)
death (d), grazing (g), and egestion (e)

Mass transfer processes are
re-aeration (re)
settling (s)
sediment oxygen demand (sod)
sediment-water exchange (sw)



Model – Constituents | Mass balance

For each state variable, a mass balance is written for **each vertical layer**.

EXAMPLE: for the epilimnion (in the case where the inflow and outflow pass directly through the epilimnion) the balance is written as

$$V_1 \frac{dc_1}{dt} = Q_{in} c_{in} - Q_{out} c_1 + E_1^{'}(c_2 - c_1) + S_1 V_1$$

where

c_i = the concentration of layer i [mg/L or µg/L],

c_{in} = the concentration of the inflow [mg/L or µg/L]

E_i' = the bulk turbulent diffusion coefficient across the lower boundary of layer i [m^3/d]

S_i = sources and sinks of the constituent due to reactions and mass transfer mechanisms [g/m^3/d or mg/m^3/d].

Similar balances are written for the other layers.

Model – Constituents | biochemical reactions

- Plant Photosynthesis (C, O, N and P)
- Plant Respiration (C, O, N and P)
- Nitrification and Denitrification

→ Oxygen generation and consumtpion involved in all these processes

Model – Constituents | biochemical reactions

Temperature effects on reactions

With the exception of phytoplankton photosynthesis, the temperature effect for all first-order reactions used in the model is represented by the Arrhenius or "theta" model

$$k(T) = k(20)\theta^{T-20}$$

where

k(T) = the reaction rate [/d] at temperature T [°C]

k(20) = reaction rate [/d] at temperature T = 20 °C

θ = the temperature parameter for the reaction.

Model – Phytoplankton

Three phytoplankton groups can be simulated.
Since all use **identical formulations**, the following description applies to all groups.
Distinctions between the groups are represented by using **different parameter values**.

$$S_{ap} = \text{PhytoPhoto} - \text{PhytoResp} - \text{PhytoDeath} - \text{HZooGraz} - \text{PhytoSettl}$$

Phytoplankton biomass increases due to photosynthesis.
It is lost via respiration, death, grazing and settling

→ Dependance: temperature, nutrient limitation, light limitation

Model – Re-aeration formula

Three methods are used to represent the dependence of oxygen gas transfer on temperature and wind speed.

Two consist of simple formulas, whereas the third consists of a more elaborate algorithm.

- Banks-Herrera formula
- Wanninkhof formula (Wanninkhof 1991)
- O'Connor Algorithm (O'Connor 1983) default

Simulation 0

- Open:
  - L2KMaster0104R2_32bit_original.xlsm
  - L2KMaster0104R2_64bit.xlsm

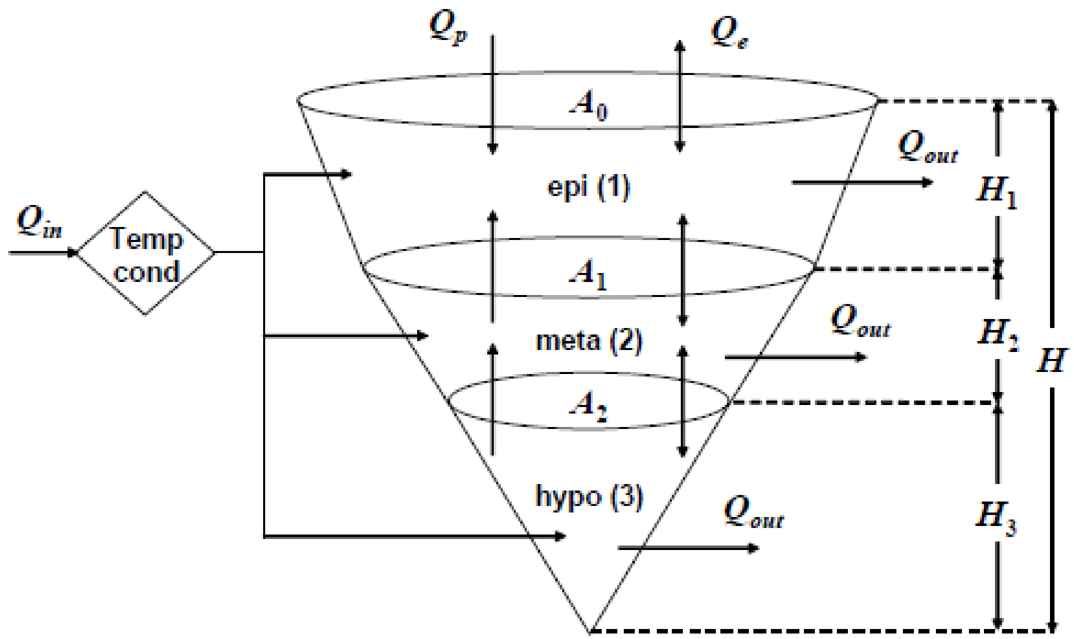
(Depending on your excel version)

Simulation 0

- Open ‘L2KMaster0104R2_32bit_original.xlsm’ or “L2KMaster0104R2_64bit” (Lake2K folder) depending on the Excel version you are running
- In ‘LAKE2K’ sheet set the *“Directory where file saved”* → select a folder in C on your pc
- RUN the model → save it as Sim_0
- In ‘Output WQ’ copy and export in another file excel the following time series:
  - Organic Nitrogen (columns Q-R-S)
  - Organic Phosphorus (columns Z-AA-AB)
  - Dissolved oxygen (columns AL-AM-AN)
  - Phytoplankton (columns AO-AP-AQ)

→ Create a chart for each time series

Simulation 1



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The volumes of the two deeper layers (metalimnion and hypolimnion) are held fixed whereas the epilimnion is allowed to change as a function of the balance between inflows and outflows.

Simulation 1

Outflow position (from Epilimnion to Hypolimnion)

- In ‘Outflow’ change the “Outflow mode” in cell B6 → Flowout(hypo)=Flowin
- In ‘Output WQ’ copy and export in another file excel the following time series:
  - Organic Nitrogen (Q-R-S)
  - Organic Phosphorus (Z-AA-AB)
  - Dissolved oxygen (AL-AM-AN)
  - Phytoplankton (AO-AP-AQ)

→ Create a chart for each time series

COMMENT ON SOLUTION
The presence of phytoplankton is reduced along the whole year. Destratification of lake: mixing phenomena are more intense because of the lower outflow position. This reflects in decreased nutrients concentration in the upper layers, higher oxygen concentration, and lower phytoplankton levels.

Simulation 2 –phytoplankton

Nutrient

RESET ALL SETTINGS TO Sim_0 conditions before doing Sim_2.

Increase the concentration of inorganic P (by 30%):

- in EPI ('initial conditions', cell B18)
- in HYP ('initial conditions', cell D18)
- in the inflow (cells V8 and V9)

COMMENT ON SOLUTION

There is a (small) increment in phytoplankton presence due to higher initial P concentration.

Simulation 3 – re-aeration

- Open Sim_0
- Run the 3 methods proposed by the tool (O'Connor, Banks-Herrera, Wanninkhof), sheet 'rates', cell B52
- Are there considerable differences in Dissolved oxygen?

COMMENT ON SOLUTION

The third method – Wanninkhof – slightly overestimates peaks. No other big differences are found.