Modeling in aquatic environment

Lecture 9

Combined water and gas models

Timo Huttula and Petri Kiuru

Timo.huttula@environment.fi

http://www.ymparisto.fi/syke/jyvaskyla

PhD work

Modelling the effect of climate change on the air-water carbon gas exchange in boreal lakes

Petri Kiuru

University of Jyväskylä, Department of Physics /

Finnish Environment Institute, Freshwater Centre

Contents

- Multi-Year Lake Simulation Model MyLake
- MyLake applications and model development
- Oxygen & dissolved inorganic carbon submodel
- CO_2 modelling: Lake Valkea-Kotinen
- Future plans
- Required data for modelling

Multi-Year Lake Simulation Model MyLake

- Multi-year simulation model for Lake thermo- and phytoplankton dynamics
- Developed at the Norwegian Institute for Water Research (NIVA)
- One-dimensional process-based model code
- Simulates
  - Lake water temperature, stratification
  - Sediment-water interaction (heat flux, sedimentation, resuspension)
  - Phosphorus-phytoplankton dynamics
  - Dissolved organic carbon (DOC) (FOKEMA module)
  - New: oxygen, dissolved inorganic carbon, carbon dioxide
- Time step 1 day, vertical layer thickness user-definable

Model input

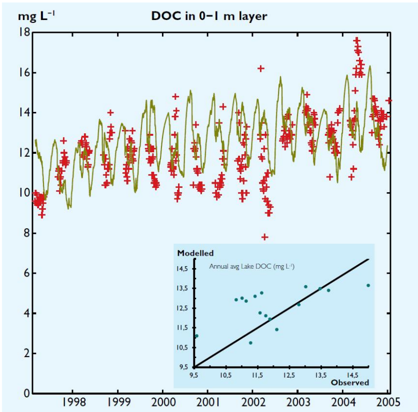
- Daily meteorological variables
  - Global radiation [MJ m^{-2} d^{-1}]
  - Cloud cover (0 - 1)
  - Air temperature [º C] at 2 m height
  - Relative humidity (%) at 2 m height
  - Atmospheric pressure [hPa] at station level
  - Wind speed [m s^{-1}] at 10 m height
  - Precipitation [mm d^{-1}]
- Daily inflow (can be excluded)
- Daily inflow concentrations of suspended matter, total phosphorus, dissolved organic phosphorus, chlorophyll, oxygen, dissolved inorganic carbon and dissolved organic carbon (can be excluded)
- Lake bathymetry, initial lake temperature and concentration profiles

MyLake applications and model development

MyLake application project at SYKE 2009-2012

- Processes controlling DOC fluxes in boreal catchments (PRO-DOC): model chain consisting of a hydrological model (HBV), a catchment model for carbon (INCA-C) and MyLake
- Lake Valkea-Kotinen
- MyLake submodel (FOKEMA) for microbial and photochemical degradation of dissolved organic carbon

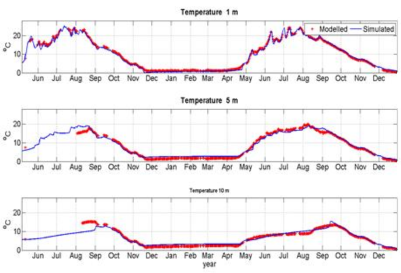
Holmberg M. et al. 2014. Effects of changing climate on the hydrology of a boreal catchment and lake DOC – probabilistic assessment of a dynamic model chain. *Boreal Env. Res.* 19 (suppl. A): 66–82.



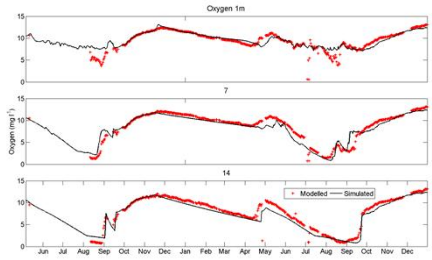
MyLake applications and model development

MyLake application project at the University of Jyväskylä 2011-2012

- CLEEN MMEA (Measurement, Monitoring and Environmental Assessment), Lake Jyväsjärvi: operative lake temperature and oxygen forecast model
  Predicting the development of vertical temperature on the basis of meteorological forecast data: a 5-day forecast (www.paijanne.org)



•Temperature calibration June 2010 – December 2011

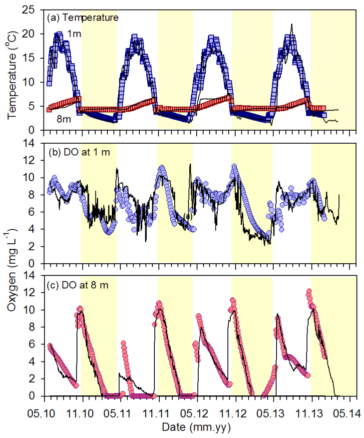


•Oxygen calibration June 2010 – December 2011

MyLake applications and model development

MyLake application at Norwegian Institute for Water Research (NIVA) 2013-

- Couture et al. *Oxygen dynamics in a boreal lake responds to long-term changes in climate, ice phenology and DOC inputs.* Submitted manuscript
- Lake Langtjern, Norway
- The new oxygen submodel is utilized in the application



•Temperature & oxygen calibration 2010 – 2014

Physical model

- Heat conservation equation for temperature distribution in a horizontally homogenous, vertically stratified lake

$$A\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[KA\frac{\partial T}{\partial z}\right] + A\frac{Q''}{\rho_w C_p}$$

- Vertical diffusion coefficient *K* is estimated from the Brunt-Vaisala frequency N^2:

$$N^2 = \frac{g}{\rho_w}\frac{\partial \rho_w}{\partial z} \qquad K = a_k (N^2)^{-0.43} \qquad a_k = 0.00706(A_s)^{0.56}$$

- Local heating during open water period for the surface layer: water-sediment heat flux + turbulent (latent and sensible) heat flux + net longwave r ... rmulas from MATLAB

$$\Delta T_1 = (Q_{WS\_norm\_1} + Q_{turb} + Q_{lw} + Q_{sw\_abs\_1})A_1 / \rho_w C_p V_1$$

$$\Delta T_{i>1} = (Q_{WS\_norm\_i} + Q_{sw\_abs\_i})A_i / \rho_w C_p V_i$$

- For subsurface layers

Physical model

- The processes here are solved in sequence i.e. are applied to the lake system once a day.
- Convective mixing: all layers with unstable density profile are mixed with the first stable layer below the unstable layers.
- Wind-forced mixing: available kinetic energy *TKE*, wind sheltering factor W_{str}

$$TKE = W_{str} A_s \sqrt{\frac{\tau^3}{\rho}}\Delta t \qquad W_{str} = 1.0 - \exp(-0.3 A_s)$$

- Potential energy *PE* needed to mix the first non-epilimnion layer into the epilimnion

$$PE = g\Delta\rho_w \frac{V_{epi}V_z}{V_{epi}+V_z}(z_{epi} + \Delta z_{M\_z} - z_{M\_epi})$$

->The process is continued until the kinetic energy is consumed

Physical model

- River inflow is added to the top of the first water layer heavier than the inflow, and the water column above the inflow level is ”lifted” according to the volume of the inflowing water. The part which is ”lifted” above the surface level is considered as the outflow.

- Ice growth from Stefan’s law:

$$h_{ice\_new} = \sqrt{{h_{ice}}^2 + \frac{2\kappa_{ice}}{\rho_{ice} L}(T_f - T_{ice})\Delta t}$$

- The water flooding on top of the ice mixes with the lower part of the snow an forms a slush layer which becomes snow ice when frozen.
- Snow density value is updated at the end of each time step
- All snow must melt before ice surface melting can start.

(Start)

For one model time step (24 h):

- Calculate daytime surface heat fluxes and wind stress, light attenuation, and phytoplankton growth and loss rates. Calculate also the heat flux between water and sediment.
- Apply daytime heat sources, allow convection, calculate nighttime surface heat sources and apply them, allow convection.
- Calculate profile of the diffusion coefficient K
- Solve new profile for each state variable taking into account advection, diffusion and local sources/sinks. Solving is done in following order: 1) temperature (after which convection is allowed), 2) tracer, 3) dissolved inorganic phosphorus (P_{DO}), 4) suspended inorganic particulate matter (S) and associated particle bound phosphorus (P_{IP}), 5) chlorophyll *a* (P_{Chla}), 6) dissolved phosphorus (P_D), 7) dissolved inorganic carbon (DOC).
- Update phosphorus concentration in the sediment (exchange between pore water and water column, net sedimentation and burial to inactive layer, partitioning of phosphorus between dissolved and particle bound phases).
- Add river inflow and update profiles of the state variables accordingly. Allow partitioning of phosphorus between dissolved and particle bound phases, as well as convection.

    If no ice

    - ❑ Mix water layers with the available turbulent kinetic energy from wind.

    If ice cover

        If $T_a < T_f$ *(freezing)*

        - ♦ Calculate ice surface temperature (depending on snow cover, or ice thickness if snow is absent)
        - ♦ Calculate snow ice formation in case of isostatic imbalance
        - ♦ Calculate congelation ice growth by Stefan’s law
        - ♦ Accumulate new snow fall and subtract formed snow ice from snow cover

        If $T_a \geq T_f$ *(melting)*

        - ♦ Melt snow or ice from top with total surface heat flux

    - ❑ Melt ice from bottom with the heat diffused to the surface layer (keeping the surface layer temperature at freezing point)
    - ❑ Update snow density

- Allow partitioning of phosphorus between dissolved and particle bound phases in the water column.
- Check the water column for supercooled layers and turn them into initial ice cover.
- Save results to output matrices.

(Goto Start)

Oxygen & dissolved inorganic carbon submodel

- Description of dynamics of oxygen and dissolved inorganic carbon in MyLake
  - Photosynthetic oxygen production / carbon dioxide consumption
  - Biological oxygen demand and sediment oxygen demand
  - Oxygen & carbon dioxide exchange between lake water and atmosphere

Oxygen & dissolved inorganic carbon submodel

Dissolved inorganic carbon production and consumption

•Carbon dioxide and oxygen concentrations are governed by growth and loss of phytoplankton, biological oxygen demand sediment oxygen demand and surface flux

•Carbon dioxide production is connected to oxygen consumption:

$$\Delta CO_2 = -\frac{M_{CO2}}{M_{O2}}\Delta O_2 = -\frac{M_{CO2}}{M_{O2}}\left(A(\Delta P_{Chla} + \Delta P_{Chl}) - (\Delta O_{2,BOD} + \Delta O_{2,SOD})\right)$$

•where *A* is a stoichiometric constant, P_{Chla} and P_{Chl} are phytoplankton (chlorophyll *a*) concentrations, $\Delta O_{2,BOD}$ is the change in oxygen concentration due to bioloxical oxygen demand ja $\Delta O_{2,SOD}$ is the change in oxygen concentration due to sediment oxygen demand.

•O_2–DIC model inputs: O_2 concentration (initial profile, inflow), DIC concentration (initial profile, inflow) and pH (constant 5.2 in Valkea-Kotinen).

•O_2 and DIC go through the same diffusive, convective and wind mixing processes as the other variables.

•Output variables: O_2 [mg/m^3], DIC [mg/m^3] and CO_2 [mmol/L].

Oxygen & dissolved inorganic carbon submodel

Fractionation of dissolved inorganic carbon in water

- Dissolved inorganic carbon DIC includes carbon dioxide $(CO_2)_{aq}$, carbonic acid H_2CO_3, carbonate HCO_3^- and bicarbonate CO_3^{2-}.
- The equilibria that control the carbon dioxide fraction in the solution are

$$(CO_2)_g \overset{K_0}{\leftrightarrow} (CO_2)_{aq}$$

$$(CO_2)_{aq} + H_2O \overset{K_H}{\leftrightarrow} H_2CO_3$$

$$(CO_2)_{aq} + H_2O \overset{K_1}{\leftrightarrow} H^+ + HCO_3^-$$

$$HCO_3^- \overset{K_2}{\leftrightarrow} H^+ + CO_3^{2-}$$

- The sum of the concentrations of $(CO_2)_{aq}$ and H_2CO_3 is used in the model and it is denoted by CO_2

Oxygen & dissolved inorganic carbon submodel

Fractionation of dissolved inorganic carbon in water

- Solubility coefficient of carbon dioxide in water K_0 [mol kg^{-1} atm^{-1}] (Millero 1995)

$$K_0 = \exp\left(-60{,}2409 + 93{,}4517\left(\frac{100}{T}\right) + 23{,}3585 \ln \frac{T}{100}\right)$$

  where T is water temperature [K].
- Dissociation constant of bicarbonate and carbonate [mol kg^{-1}]

$$K_1 = \exp\left(290{,}9097 - 14554{,}21\left(\frac{1}{T}\right) - 45{,}0575 \ln T\right) \qquad K_2 = \exp\left(207{,}6548 - 11843{,}79\left(\frac{1}{T}\right) - 33{,}6485 \ln T\right)$$

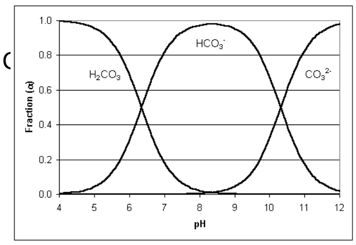
- Hydrogen ion concentration

$$[H^+] = 10^{-\mathrm{pH}}.$$

  Currently pH = constant.
- Fraction of carbon dioxide [mol CO_2 / mol DIC

$$[CO_2]_{aq} = f_{CO2}^{DIC} C_{DI},$$

$$f_{CO2}^{DIC} = \frac{[H^+]^2}{[H^+]^2 + K_1[H^+] + K_1 K_2}.$$



Oxygen & dissolved inorganic carbon submodel

Air-water carbon dioxide exchange

•Carbon dioxide flux *F* on the surface [mmol/m^2 d] (Cole & Caraco 1998)

$$F = \alpha k CO_2([CO_2]_{sur} - [CO_2]_{eq}),$$

where α (= 1) is the chemical enhancement factor, $[CO_2]_{sur}$ is the CO_2 concentration in the surface water and $[CO_2]_{eq}$ the CO_2 equilibrium concentration

•Gas transfer velocity [cm/h] for carbon dioxide (Jähne et al. 1987)

$$kCO_2 = k_{600}\left(\frac{ScCO_2}{600}\right)^{-0,5}$$

•The transfer velocity for Schmidt number 600 (Cole & Caraco 1998)

$$k_{600} = 2,07 + 0,215w^{1,7},$$

where *w* is wind speed at 10 meter height [m s^{-1}],

and the Schmidt number for carbon dioxide is (Wanninkhof 1992)

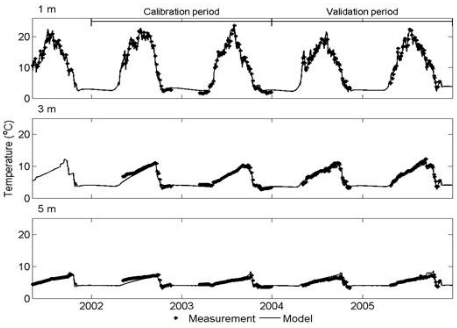
$$ScCO_2 = 1911,1 - 118,11T_0 + 3,4527T_0^2 - 0,041320T_0^3,$$

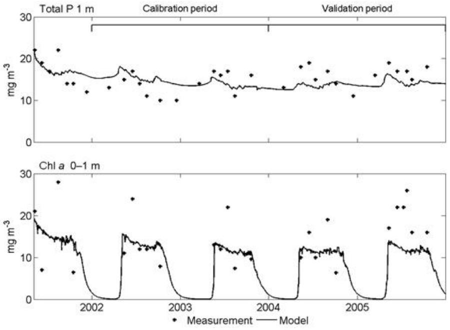
where T_0 is the surface water temperature

Oxygen-DIC model application in Lake Valkea-Kotinen

Kiuru P., Ojala A., Mammarella I. & Huttula T. *A process-based model for simulation of lake oxygen and DIC.* Manuscript.

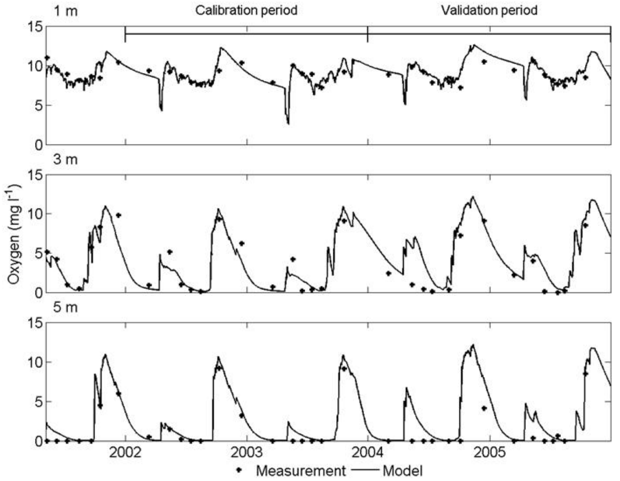
- Meteorological forcing , surface discharge and lake temperature time series from PRO-DOC data
- Discharge TotP from the WSFS-Vemala model
- Lake TotP, Chla, O_2 from HERTTA database
- Calibration period 2002-2003, validation period 2004-2005
- Layer thickness 0.5 m





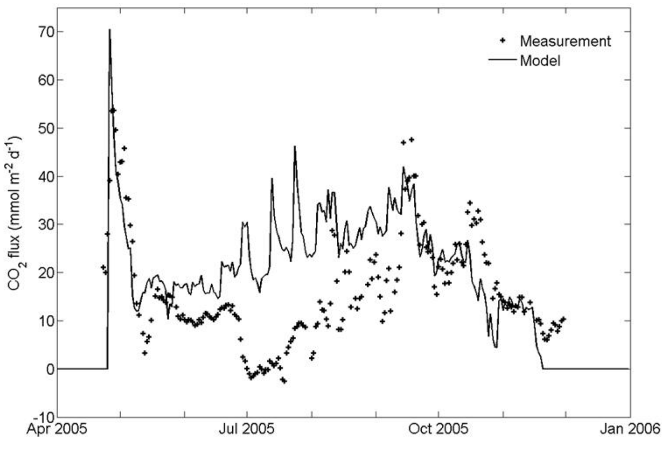
Oxygen-DIC model application in Lake Valkea-Kotinen

- Dissolved oxygen 2001-2005



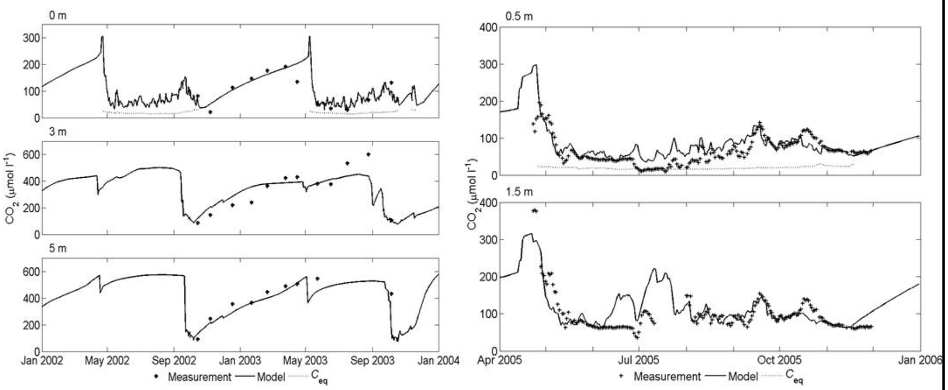
Oxygen-DIC model application in Lake Valkea-Kotinen

- Carbon dioxide surface flux in 2005



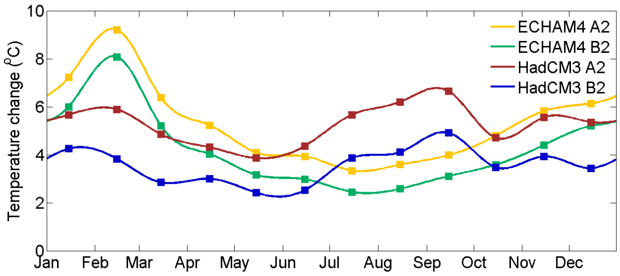
Oxygen-DIC model application in Lake Valkea-Kotinen

- Carbon dioxide concentration in 2003 and 2005



Climate change scenarios

- Climate change scenarios relative to the baseline period 1961–1990 for locations in Finland: FINSKEN (www.finessi.info/finsken)
  - SRES greenhouse gas emissions scenarios A2 & B2



22

Climate change scenarios

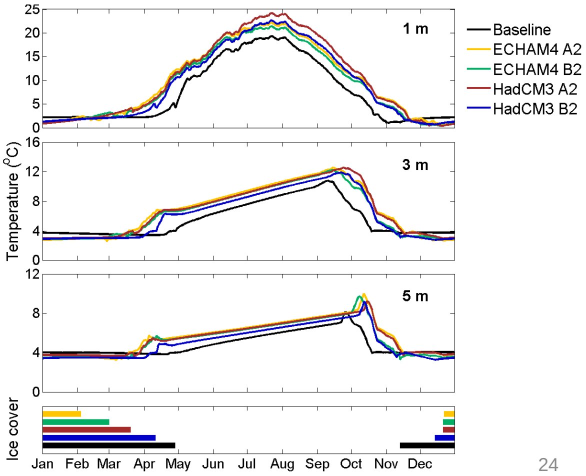
- Baseline period:
  - Daily average of meteorological forcing and discharge loading in 1990–2005
- Scenario period:
  - Daily air temperature change interpolated from monthly change from CGM results
  - Inflow temperature estimated from air temperature
  - No change in discharge

23

Scenario results

Temperature 1990–2005 vs. 2071–2100

- Stronger stratification
- Little change in thermocline depth due to physical effects
- 50–120 d longer ice-free period

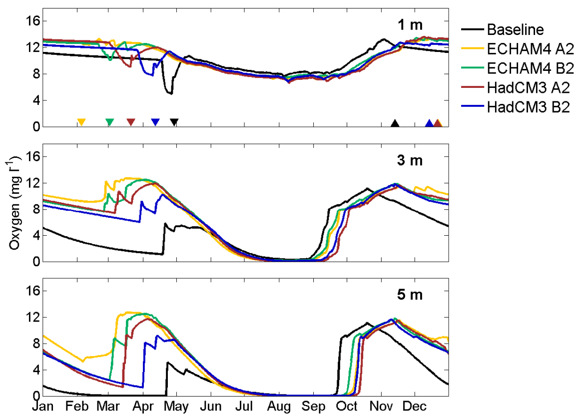


24

Scenario results

Dissolved oxygen 1990–2005 vs. 2071–2100

- Longer mixing period after ice melt → longer anoxia only in late summer
- Shorter ice season → no anoxia in winter

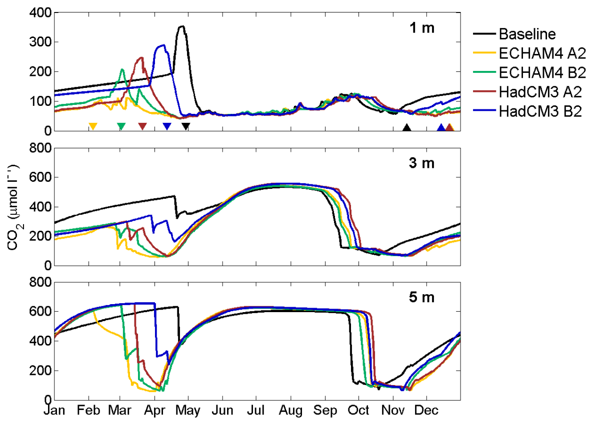


25

Scenario results

Carbon dioxide 1990–2005 vs. 2071–2100

- Shorter ice season → less accumulation under ice

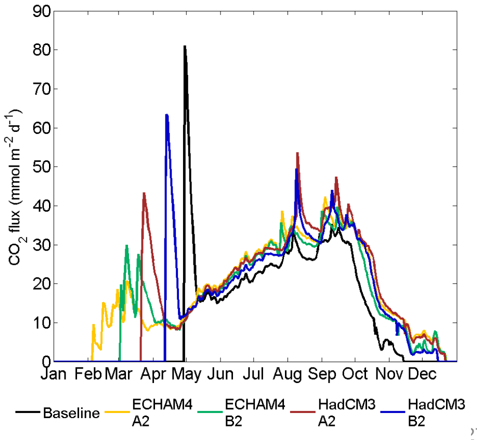


26

Scenario results

Carbon dioxide flux 1990–2005 vs. 2071–2100

- Lower spring peak
- Higher overall level
- Yearly flux to the atmosphere +25...40 %



27

Conclusions

- Modelling is an efficient tool in assessing the impacts of climate change on carbon cycle in boreal lakes
- The one-dimensional process-based model for simulation of lake dissolved oxygen and DIC gives reasonable validation results for a boreal lake
- Effects of higher air temperature on oxygen and CO_2 dynamics in L. Valkea-Kotinen
  - Longer mixing period in spring → complete turnover
  - Longer hypolimnetic anoxia in autumn
  - Greater CO_2 flux to atmosphere

28