Modelling photosynthetic function in a changing light environment – a summary of existing models

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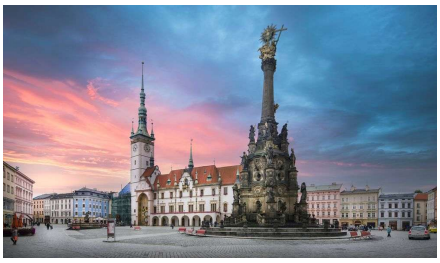
Olomouc
- the 6th largest city in Czech Republic
- the capital of Olomouc Region
- about 100 000 inhabitants



Palacký University Olomouc
- the 2nd oldest university in Czech Republic, established in 1573
- 7 faculties and 1 research institute
- over 270 bachelor´s, master´s and doctoral study programs
- about 23 000 students per year

Mathematical modelling of photosynthetic function

- structure of model depends on the goal, variables, model assumptions
- chlorophyll fluorescence (ChlF) is very often measured and thus modeled
- the models were mostly used for simulation of ChlF during transient from dark to **constant light** (ChlF induction)

- first models were very simple, e.g., 4 ordinary differential equations (**ODE**s) for electron transport between Q_A and the PQ pool (Malkin 1966, Munday and Govindjee 1969)

- in present days, models can be very complicated, e.g., 386 ODEs for PSII only (Lazar 2013)

- whole electron transport in the thylakoid membrane (e.g., Lebedeva et al. 2002, Kroon and Thoms 2006, Lazar 2009, Zaks et al. 2012, Beleaeva et al. 2013)

- also enzymatic reactions in stroma (Calvin-Benson-Bassham (CBB) cycle) and cytosol (Laisk et al. 2006, 2009, Zhu et al. 2013)

Summary: „everything“ (for illumination by constant light intensity) was modelled and in different levels of details

Goal: summary of processes considered in modeling of photosynthesis under changing light environment

How to determine what should be considered in the model:
- seek for regulatory processes and their time (rate) constants
- look at the literature how it has already been done before

Changing light environment means:
- flashing light
- pulsed light
- intermittent light
- dynamic light
- light-dark cycle
- fluctuating light
- oscillating light

Models according to their complexity:

I – Models based on description of the light-dependent reactions and CO_2 assimilation reactions
simple and more complicated

II – Models based on description of the CO_2 assimilation reactions and stomata function
simple and more complicated

III – Simple models based on description of the photoacclimation and photoinhibition

IV – Models based on description of the non-photochemical quenching
simple and more complicated

V – Complex models

VI – Our models (BDM and BDM2)

VII – Models for the spontaneous oscillations

VIII – Data-driven models – systems identification

I – Models based on description of the light-dependent reactions and CO_2 assimilation reactions – SIMPLE 1

Thornley (1974) -> **Gross (1982)**

- probably the first ever model for photosynthesis under dynamic light
- no experiments, theoretical analyses only
- model finally resulted in **1 ODE** for **rate of photosynthesis** (P) with six parameters:

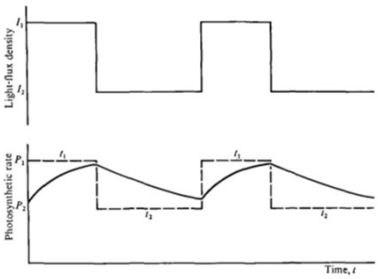
$$\frac{dP}{dt} = hk_2k_1X_oCI - k_1IP - k_2CP$$

- further improved by one ODE for **rate constant of formation of the active photosynthetic intermediate** to:

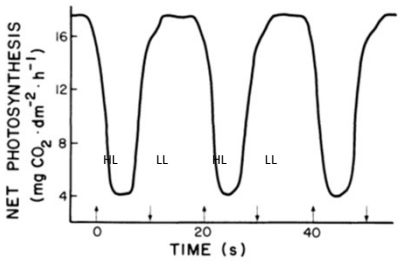
$$\frac{dP}{dt} = \frac{1}{\gamma}[K_2K_1(t) - (K_1(t) + K_2)P(t)]$$

$$\frac{dK_1}{dt} = \frac{1}{R(\ell_t)}[\bar{K}_1L(t) - K_1(t)]$$

where R is a complicated phenomenological function of history of sample illumination



Thornley (1974, Ann. Bot.)

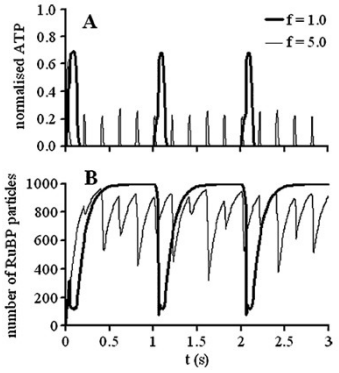


Gross (1982, Ecology)

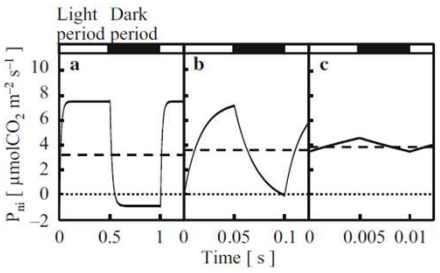
I – Models based on description of the light-dependent reactions and CO_2 assimilation reactions – SIMPLE 2

Yoshimoto et al. (2005), Jishi et al. (2015)

- to describe the flashing light effect (FLE) = „enhancement“ of photosynthesis in algae grown under flashing light
- models are **algebraic equations**, one for **the light dependent reactions** and one for **the CO_2 assimilation reactions**:
- for **ATP** or for **fraction of reduced pool of electron carriers** (Q_A, PQ, NADPH)
- for **RuBP** or for **rate of CO_2 assimilation**, which depends on the light-dependent reaction



Yoshimoto et al. (2005, Photosyn. Res.)



Jishi et al. (2015, Photosynth. Res.)

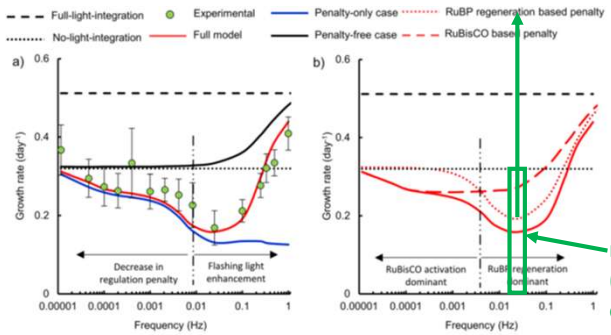
I – Models based on description of the light-dependent *reactions* and CO_2 assimilation reactions – MORE COMPLICATED

Graham et al. (2017), Salvatori et al. (2022)

- to describe photosynthesis of cyanobacteria and algae under different frequencies of light duty cycles with different duty cycle ratios and of soybean varieties under low/high light cycles

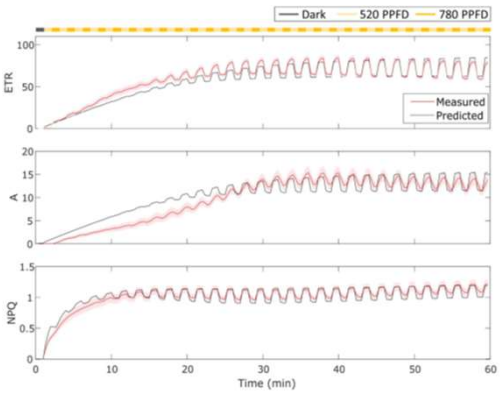
- light-dependent reactions: **2 ODEs** for reversible light-induced transition of **resting PSU to their active state**
- CBB cycle: **4 ODEs**, 2 for **reversible regeneration of RuBP** and 2 for **reversible Rubisco activation**

- light-dependent reactions: **4 independent ODEs** for PSII energization, activation level of NPQ related proteins, quenching complex of the energized PSII with activated NPQ proteins, NADPH
- CBB cycle: **1 ODE** for Rubisco activation



Graham et al. (2017, Sci. Rep.)

resonance range (1/30 s – 1/60 s) in our experiments!



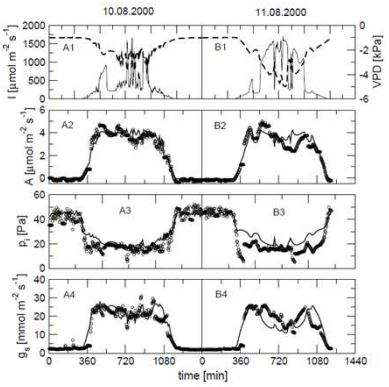
Salvatori et al. (2022, Front. Plant Sci.)

II – Models based on description of the CO_2 assimilation reactions and stomata function – SIMPLE

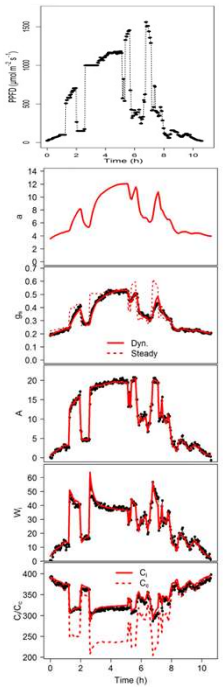
Noe and Giersch (2004), Vialet-Chabrand et al. (2016), Joubert et al. (2023)

- to describe photosynthesis of oak, Arabidopsis and tomato leaves, respectively, under fluctuating light
- models have **3, 4, and 2 ODEs**, respectively, for:

- leaf (stomatal) conductance (g_s), CO_2 partial pressure in leaf (p_i), pool of CBB cycle intermediates (a_{ps}), carboxylation rate is feedback inhibited by the pool
- stomata pore area (a), CO_2 concentration in intercellular spaces (C_i), CO_2 concentration in site of carboxylation (C_c), efficiency of stomatal pore area (L), which was regulated by the rate of accumulation and export of CBB cycle sugars
- total stomatal conductance (g_{tc}, inspired by Vialet-Chabrand et al. 2016), CO_2 concentration inside leaf (c_i), which included parameters calculated by the Farquhar-von Caemmerer-Berry algebraic model (Farquhar et al. 1980) with omitted limitations by the rate at which triose phosphates are utilised, the rate of CO_2 assimilation modelled by algebraic equation as a net flux of CO_2 that enters the leaf using the variables described by the 2 ODEs



Noe and Giersch (2004, Funct. Plant Biol.)

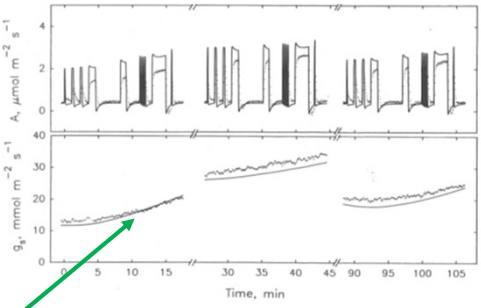


Vialet-Chabrand et al. (2016, Plant Sci.)

II – Models based on description of the CO_2 assimilation reactions and stomata function – MORE COMPLICATED

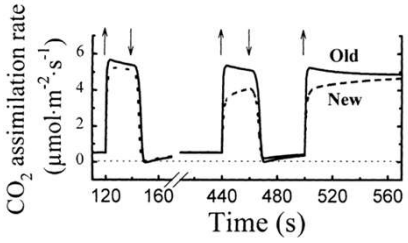
Gross et al. (1991) -> Pearcy et al. (1997) -> Kirschbaum et al. (1998)

- to describe photosynthesis under fluctuating light
- carbon cycle: **3 ODEs** for:
  - pool of reduced CBB cycle intermediates (R; RuBP), pool of glycolate pathway (photorespiration) intermediates (G), rate of carboxylation (V_{car})
- stomatal conductance: **3 ODEs** (according to Kirschbaum et al. 1988) for:
  - a biochemical signal (substance) in stomata (S), osmotic potential (π), water content in stomata (w)
- carbon cycle: **addition of 2 ODEs** for:
  - pool of precursors to R in CBB cycle (T; TP), rate of R regeneration (V_f)
- V_f was characterised by two different values of the rate constants in the same way as used for rate of carboxylation



Gross et al. (1991, Plant Cell Environ.)

stomata change conductance slowly!



Kirschbaum et al. (1998, Planta)

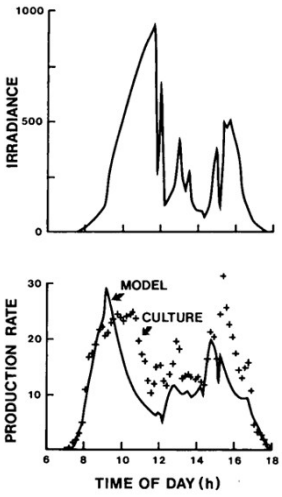
III – Simple models based on description of the photoacclimation and photoinhibition

- phytoplankton research
- *in vivo*, vertical mixing of the cells deep inside water (dark-acclimated cells) occurs with cells in the illuminated water surface (light-acclimated cells) => photoacclimation.
- in a photobioreactor, the cells can be photoinhibited in the illuminated part of the photobioreactor and then move in a cycle to a dark part of the photobioreactor => photoinhibition.

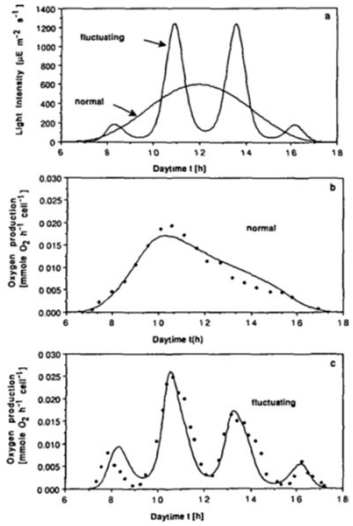
- the first model of this type was algebraic model (**Denman and Marra 1986)**

- followed by ODE-based models with **2 ODEs (Pahl-Wostl and Imboden 1990)** and **3 ODEs (Eilers and Peeters 1993, Wu and Merchuk 2001)**

- further elaborated and refined in several following papers, starting by **Camacho Rubio et al. (2003)**, going to nowadays when exploring the FLE (e.g., **Diotto et al. 2022; Sacardo et al. 2024**)



Denman and Marra (1986, Els. Ocean. Ser.)



Pahl-Wost and Imboden (1990, J. Plankt. Res.)

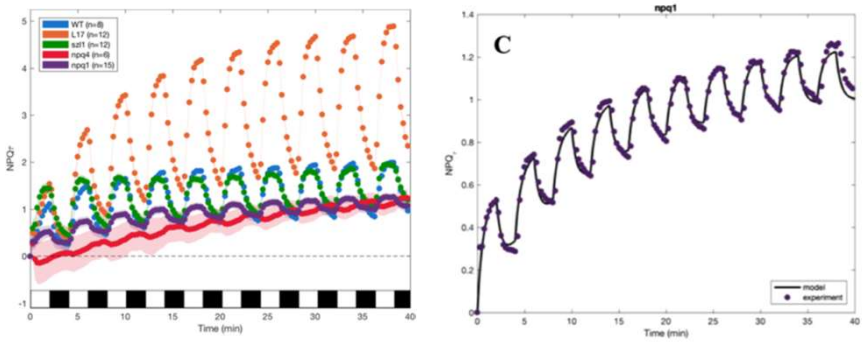
IV – Models based on description of the non-photochemical quenching – SIMPLE

Steen et al. (2020)

- Arabidopsis WT and NPQ mutants
- 2 min dark, 2 min light cycle
- ChlF lifetime snapshots
- NPQ_τ calculated from average lifetime
- active quencher (=NPQ_τ) modelled by **1 ODE**:

$$\frac{dq^{active}}{dt} = -[k_1(t) + k_2(t)]q^{active} + k_2(t)$$

where the rate constants were complicated functions of 10 parameters



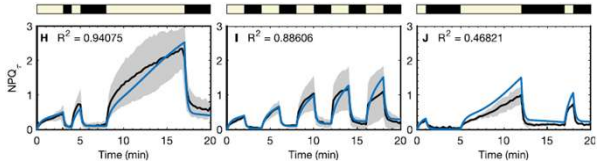
Steen et al. (2020, J. Phys. Chem.)

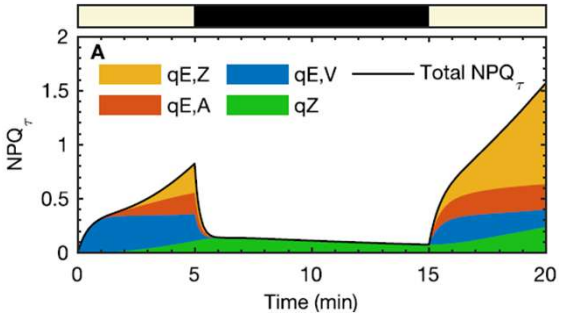
IV – Models based on description of the non-photochemical quenching – MORE COMPLICATED

Short et al. (2022) -> Short et al. (2023)

- alga *Nannochloropsis oceanica*, it has LHCX1 instead of LHCSR3 or PsbS
- ChlF lifetime snapshots, NPQ_τ calculated from average lifetime
- models:
- xanthophyll cycle but omits antheraxanthin
- 8 ODEs with 15 rate constants

- full xanthophyll cycle
- all xanthophylls (V, A, Z) can quench when in complex with protonated LBCX1 - qE(V), qE(A), qE(Z))
- Z alone can cause quenching - qZ
- 12 ODEs with 28 parameters





Short et al. (2023, Nat. Comm.)

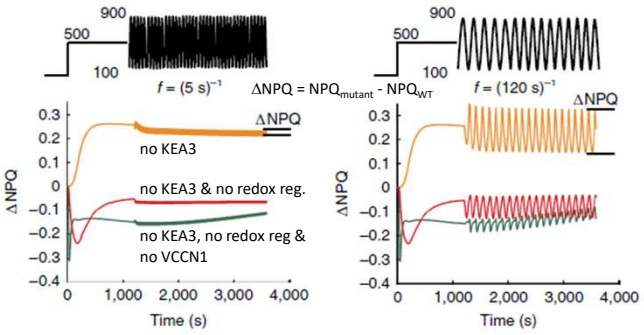
V – Complex models 1

Davis et al. (2016) -> Li et al. (2021)

- continue on previous models (Cruz et al. 2001, Zaks et al. 2012)

- theoretical study only, goal – hacking pmf partitioning to improve photosynthesis in dynamic light since the two parts of pmf affects photosynthesis differently (ΔpH -> NPQ x $\Delta\Psi$ -> FRIP)
- model:
- light-dependent reactions with emphasis on the role of counter-ions balancing light-induced lumen acidification
- only KEA3 H^+/K^+ antiport channel in TM

- model:
- added a voltage dependent K^+ channel
- added CLCe H^+/Cl^- antiport channel
- added voltage-dependent VCCN1 channel
- altogether 12 ODEs



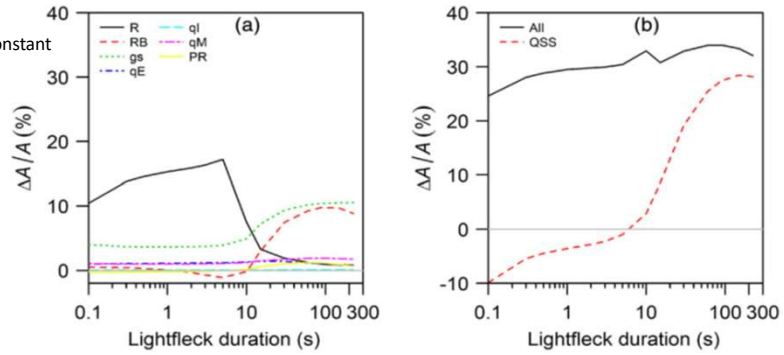
Li et al. (2021, Nat. Com.)

V – Complex models 2

Morales et al. (2018)

- 12 ODEs with 99 parameters
- 1 ODE for chloroplast movement to account for absorbance changes
- 2 ODEs (for protonated PsbS, and for zeaxanthin) for NPQ
- 3 ODEs (for PGA, RuBP, and rate constant of Rubisco activation) for function of the CBB cycle
- 1 ODE for photonhibited PSIIs
- 3 ODEs (CO_2 concentration in cytoplasm, CO_2 concentration in stroma, stomatal conductance) for gas exchange
- 2 ODEs (for CO_2 and water vapor in the measuring cuvette) to account for a delay in the measured CO_2 assimilation rate and stomatal conductance from those ones in the leaves

- virtual mutants with 1 000 000 times increased rate constant
- simulation for 30 min
- lightfleck duration has duty cycle ratio 0.5
- Intensity change from 50 to 1050 µE m^{-2} s^{-1}
- relative change (mutant – WT) of CO_2 assimilation rate



Morales et al. (2018, Plant Cell Environ.)

VI – Our models – Basic DREAM Model – BDM

Fuente et al. (2024)

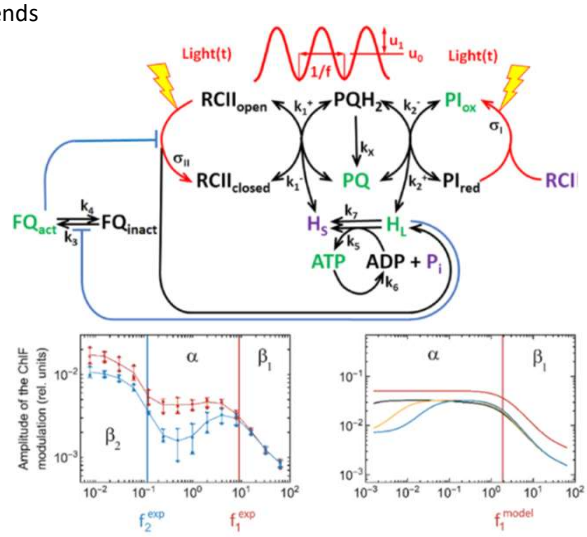
Goal: to construct a model with a regulation (represented by NPQ in the model) that would describe experimental data obtained under oscillating light

- PSII ($RCII_{open}$ and $RCII_{closed}$) assumed to be in a steady state – it depends on PQ pool, active quencher and light intensity

- set of 5 independent ODEs for (all in green):
- oxidised PQ pool (per PSII)
- concentration of protons in lumen
- oxidised donors to PSI (per PSII)
- concentration of ATP
- active quencher of excitation energy (per PSII); only one!

- 3 parameters assumed to be constant (all in violet):
- concentration of protons in lumen
- concentration of inorganic phosphate
- „photoactive“ RCI (per PSII)

- 2 output variables:
- ChlF and rate of O_2 evolution
- both depend on PQ pool, active quencher and light intensity



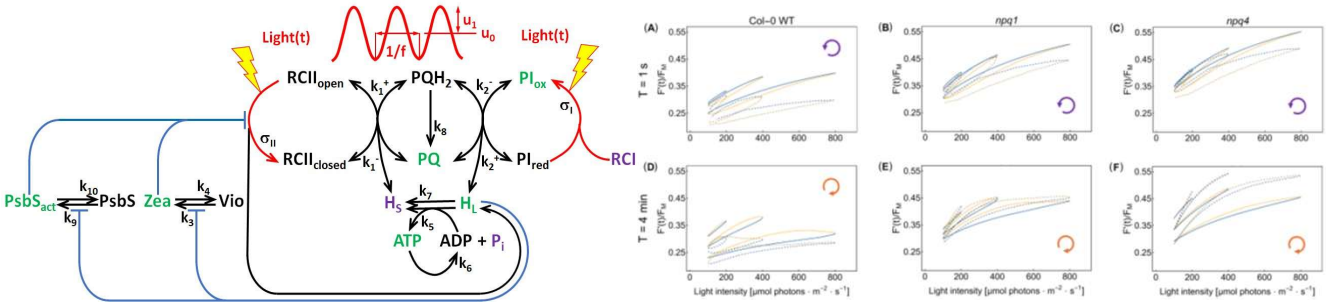
Fuente et al. (2024, Plant Physiol. Biochem.)

VI – Our models – BDM2

Niu et al. (2025)

Goal: to describe different responses of the npq1 and npq4 Arabidopsis mutants obtained under oscillating light

- one active quencher of BDM replaced by active PsbS and zeaxanthin in BDM2

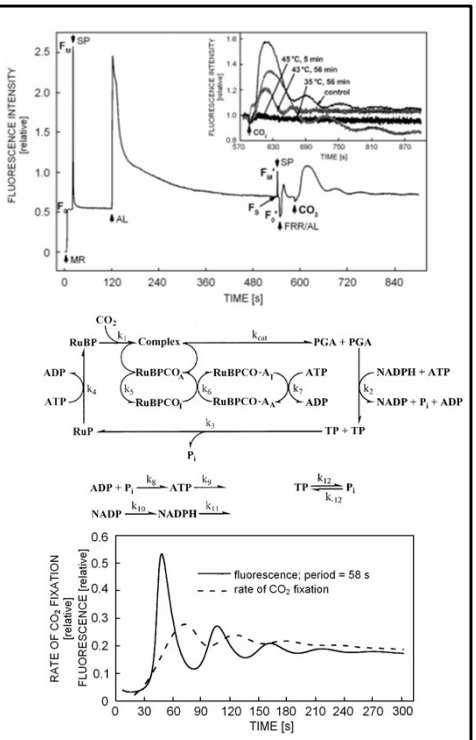


Niu et al. (2025, Physiol. Plant.)

VII – Models for the spontaneous oscillations

Several hypotheses for the source (oscillophore) of the oscillations:
- the insufficiency of ATP caused by competition for ATP between 3-phosphoglycerate kinase (PGK) and ribulose-5-phosphate kinase (RPK) during CBB cycle (Walker et al. 1983)
- concentration of orthophosphate (Pi) (Walker and Sivak 1985, Sivak and Walker 1986)
- feedback inhibition of cytosolic fructose 1,6-bisphosphate phosphatase (FBPase) by fructose 2,6-bisphosphate with a delay caused by other reactions in the sucrose synthesis in cytosol (Stitt et al. 1988)
- imbalance in the supply of ATP and NADPH to Calvin cycle caused by insufficient function of the photosynthetic electron transport chain (Laisk et al. 1991)
- ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) and its activation by Rubisco-activase (Ryde-Pettersson 1991, Roussel 1998, Lazár et al. 2005)

- also mathematically modeled (Giersch 1986, Hahn 1986, Laisk and Walker 1986, 1989, Horton and Nicholson 1987, Laisk et al. 1989, Giersch and Sivak 1991, Karavaev and Kukushkin 1993, Kocks and Ross 1995, Rovers and Giersch 1995, Buschmann and Gradmann 1997, Kukushkin 1997, Laisk and Eichelmann 1998, Roussel 1998, Khuznetsova and Kukushkin 1999, Gradmann 2001, Lazár et al. 2005)

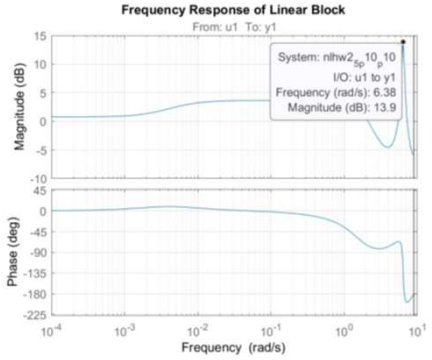


Lazár et al. (2005, Photosynthetica)

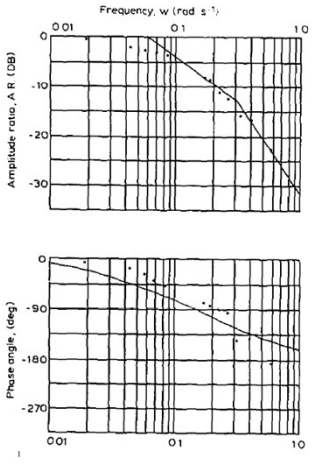
VIII – Data-driven models – systems identification

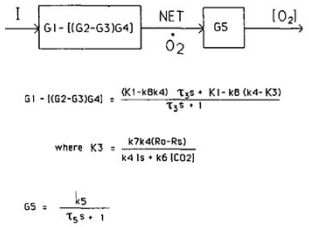
Lam and Bungay (1986)
- frequency response (1 – 1/500 Hz) of oxygen evolution of algae
- Bode plots suggest a second order system or two first-order systems in series
- a complicated block diagram of photosynthesis reduced to block diagram with two transfer functions

Bala et al. (2025)
- frequency response of ChlF of wheat plants
- Hennerstein-Wiener model
- best results with assumption of two zeros and 5 poles



Bala et al. (2025, IEEE)





$$G1 - [(G2-G3)G4] = \frac{(K1-kBk4)\ \tau_3 s + K1 - kB\,(k4-K3)}{\tau_3 s + 1}$$

$$\text{where } K3 = \frac{k7k4(Ro-Rs)}{k4\,Is + k6\,[CO2]}$$

$$G5 = \frac{k5}{\tau_5 s + 1}$$

Lam and Bungay (1986, J. Biotech.)

Conclusions

- different photosynthetic reactions were considered to model photosynthetic function in changing light environment
- in addition to NPQ, reactions related to CBB cycle seems to affect plant´s response to dynamic light and should be thus included in a new model
- some mechanism were not considered in modelling photosynthesis under changing light but these mechanisms might be important, e.g. the photosynthetic control, buffering of protons in lumen (and stroma), phosphate translocators, ..., these mechanisms should be also included in a new model

Thank you for your attention!