Transformace bilineární soustavy ODR s harmonickým buzením na soustavu PDR (*Efficient Solution of a Parameter Estimation Problem using Equation-Based Modeling in COMSOL*)

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Remembering COMSOL conference 2017 & one old (not yet resolved) problem: *How to model the fish swimming while optimizing the design of aquaculture technology?*

And now for something completely different (let see one even older problem)...

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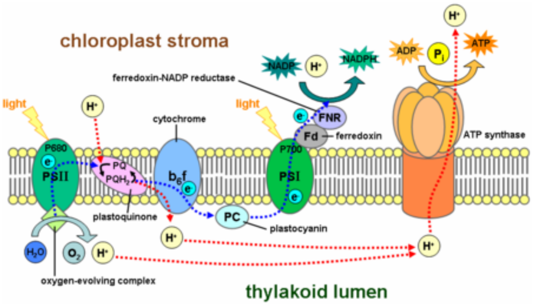
- *Exo-system* and **COMSOL Multipysics (Equation-Based Modeling)** can help !!!

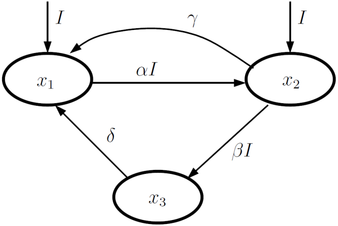
Outline

Real (micro) scale model of microalgae photosynthesis *vs.* phenomenological **model of photosynthetic factory** (PSF)



Microalgae photosynthesis in real (micro)scale: Photosynthetic protein complexes (PSII and PSI); Light and dark reactions: water splitting, CO_2 fixation, etc. vs. 3-state PSF model (please, see the next slides :)

Model calibration for **3-state 5-parameter mechanistic model of photosynthetic factory**



Stavový vektor $x = (x_1, x_2, x_3)^T$: molární frakce buněk ve stavu klidu (x_1), aktivace (x_2), resp. inhibice (x_3), tj. platí $x_1 + x_2 + x_3 = 1$. Substrátem–vstupem (řízeným) je **irradiance**–ozářenost $I(t)$.

4 parametry PSF modelu jsou "*transition rates*" α, β (in $[s^{-1}$/irrad. unit$]$), γ, δ $[s^{-1}]$. Platí $\alpha \gg \beta$, $\gamma \gg \delta$. Tzn. existence aspoň dvou časových škál (pro *světelné a temnotní reakce* a proces *fotoinhibice*).

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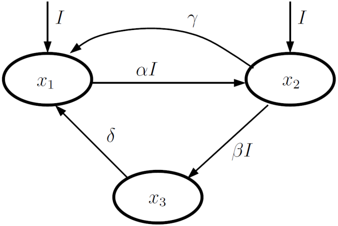

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Propojení fenomenologických stavů s reálným světem (**měřitelnou spec. růstovou rychlostí** μ) je následující (5. parametr κ):

$$\mu = \frac{\kappa\gamma}{T} \int_0^T x_2(t)\mathrm{d}t \ . \qquad (1)$$

Hodnota součinu $\kappa\gamma \approx 10^{-4}$ $[s^{-1}]$, což představuje škálový skok (ze vteřin na hodiny, tj. 3. časová škála)!

PSF: Bilineární systém s jedním (skalárním) vstupem

$$\dot{x} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & \gamma & \delta \\ 0 & -\gamma & 0 \\ 0 & 0 & -\delta \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + I(t) \begin{bmatrix} -\alpha & 0 & 0 \\ \alpha & -\beta & 0 \\ 0 & \beta & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \tag{2}$$

- IVP: "přirozené" počáteční podmínky (po inkubaci ve tmě) jsou: $x(t_0) = [1, 0, 0]^T$.
- BVP: okrajové podmínky (periodic BC) jsou: $x(0) = x(T)$.
- Pro konstantní vstup I má matice soustavy $\left[\mathcal{A} + I(t)\mathcal{B}\right]$ 2 záporná reálná vlast. čísla. Třetí vl. číslo je 0 a k němu vl. vektor je x_{ss}.

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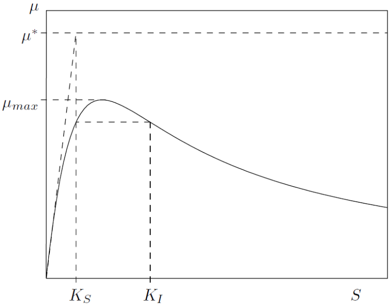
PSF model (2) vede (pro $I \equiv S = const.$) na kinetiku inhibice substrátem (SIK-Haldane: Obr. vlevo)



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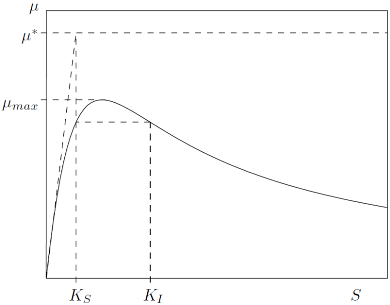
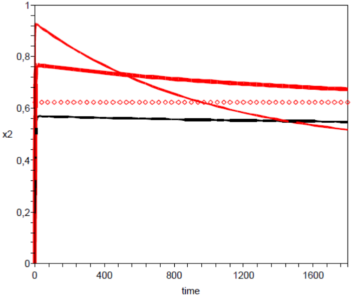




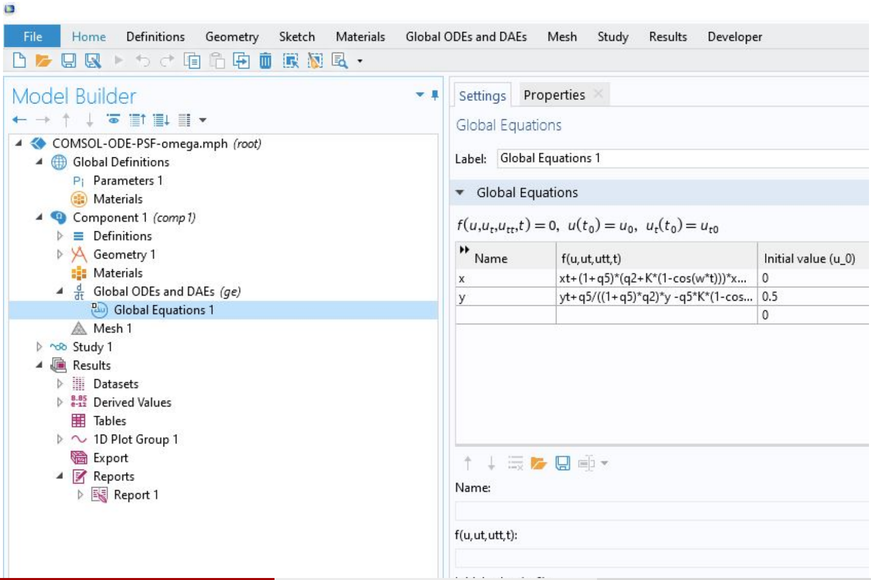
Obr. vpravo simuluje odezvu $x_2(t)$ (pro $x_2(0) = 0$) na skokovou změnu I_i, viz 2 škály.

Resumé pro kalibraci PSF modelu: 3 z 5 parametrů popisují **steady state** a 2 popisují **dynamiku**, (i) pomalou $\sim$ *photoinhibition*, (ii) rychlou (lze kalibrovat pomoci tzv. *L-D cycles* indukovaných harmonickým signálem $I(t) = K(1 - cos(\omega\ t))$, viz další sekce).

Outline

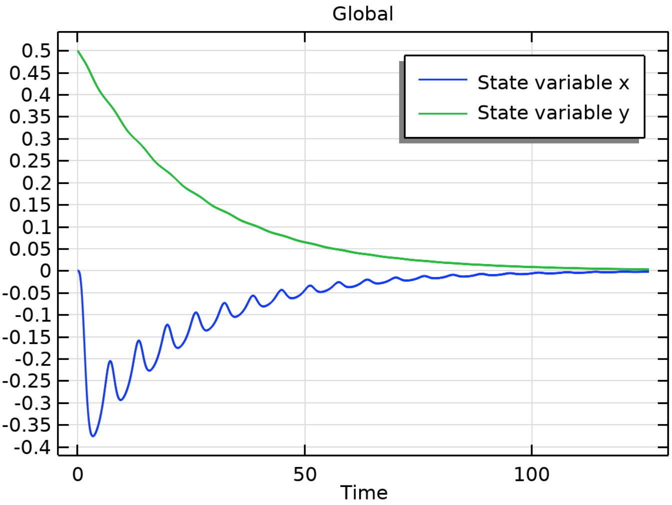
1^{st} attempt: The Global ODEs and DAEs (ge) interface

under the **Mathematics** branch *(How to set up the BVP?)*



Initial value problem gives the transient behavior...

(dependent variables transformation was used → both steady state values are 0)



How to get the periodic solution for the periodic input ?

Introducing an Exo-system as the harmonic input signal generator → ODEs are transformed to a **stationary PDE system** (4) with 2 independent and 2 dependent variables $x_2,\ x_3$.

Let us define the harmonic input as follows:
$u(t) = K(1 - \cos(\omega t)) = K(1 - w_2)$, where $w(t) = [\sin(\omega t), \cos(\omega t)]^T$.
Thus, the input signal is generated by an external autonomous system, so-called **EXOSYSTEM**.
Moreover, it holds

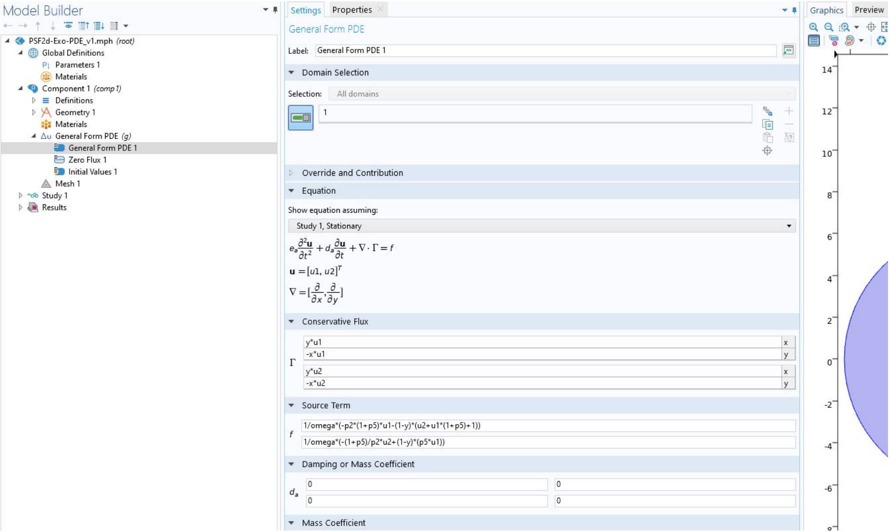
$$\dot{w}(t) = \begin{bmatrix} \dot{w}_1 \\ \dot{w}_2 \end{bmatrix} = \omega \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \omega S w, \tag{3}$$

and further

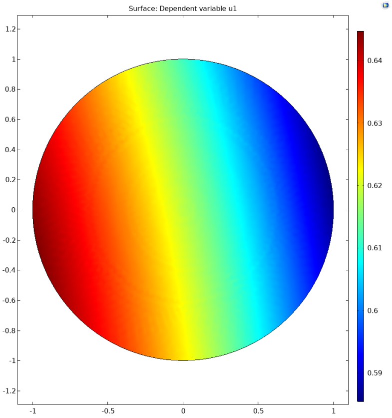
$$\dot{x} = \nabla x(w(t))\ \dot{w}(t) = \omega \nabla x(w) S w = \left[\mathcal{A} + u(w)\mathcal{B}\right] x(w), \tag{4}$$

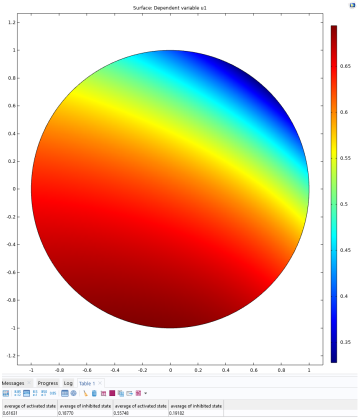
where $\nabla x := [\nabla x_1, \nabla x_2, \nabla x_3]^T$, and $\nabla x_i = [\frac{\partial x_i}{\partial w_1}, \frac{\partial x_i}{\partial w_2}]$.

2^{nd} (successful) attempt: General Form PDE interface
under the **Mathematics** branch *(2D - stationary)*



COMSOL generates simulated data (only the state x_2 is related to real world measurements)...





...and only the domain boundary is connected to the original problem...

Outline

Postprocessing of COMSOL generated data and the PSF model parameter estimation

- COMSOL generates for different ω (according to our Experimental Design) and parameters (p_i) the average values of state x_2, cf. Eq. (1).
- How to get this data? **Results-Derived Values-Line Average**.
- An optimization procedure (based on OLS method) then, find the optimal parameter values...
- ... special attention needs the "fast" parameter p_5!

Conclusion – Questions?

Thanks for your kind attention!

The ideal situation occurs when the things that we regard as beautiful are also regarded by other people as useful.

– Donald Knuth