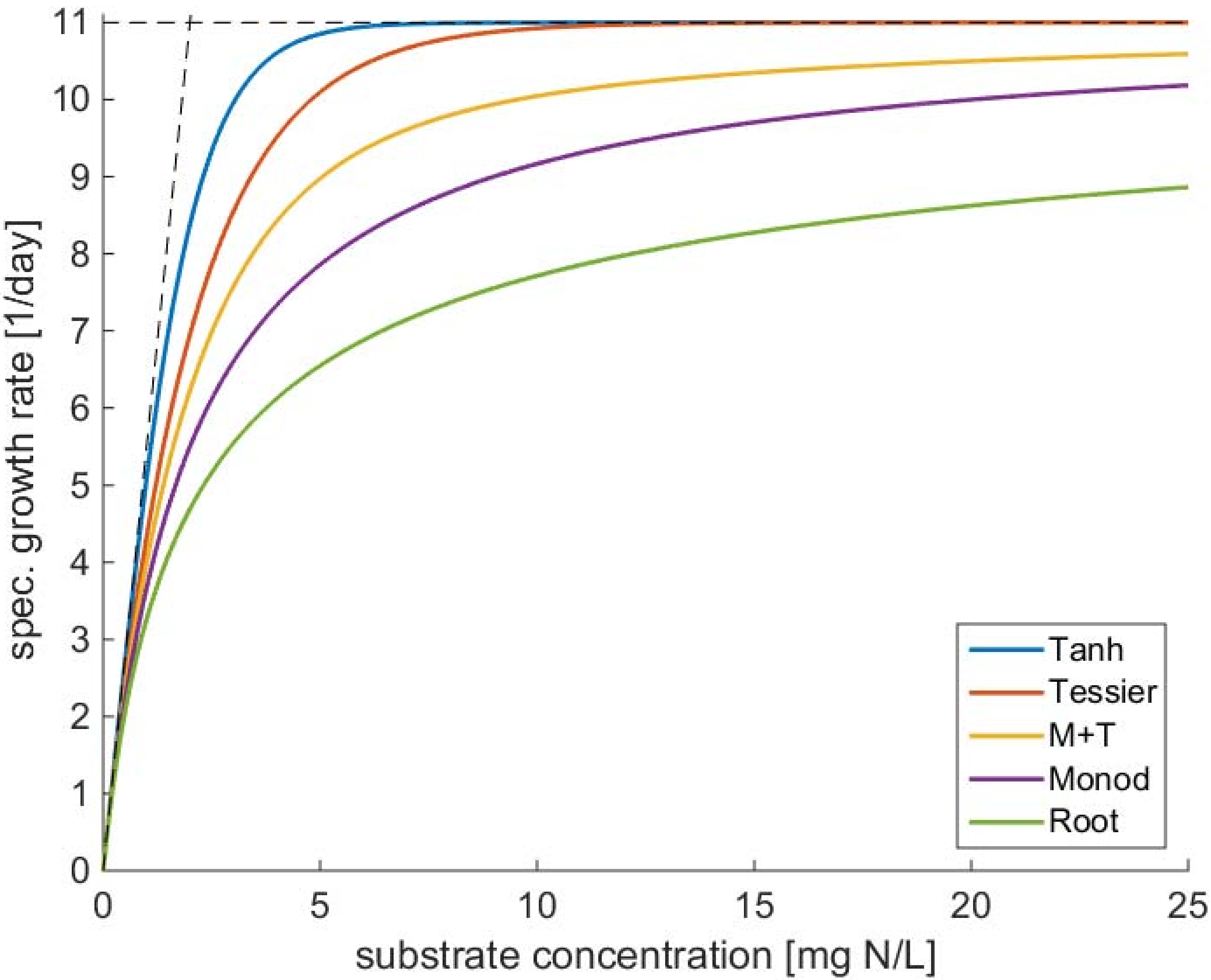
# Biokinetic process model diagnosis with shape-constrained spline functions

A. Mašić[1], S. Srinivasan[2], J. Billeter[2], D. Bonvin[2], K. Villez[1]

28 June 2016

Eawag: Swiss Federal Institute of Aquatic Science and Technology

# Problem statement

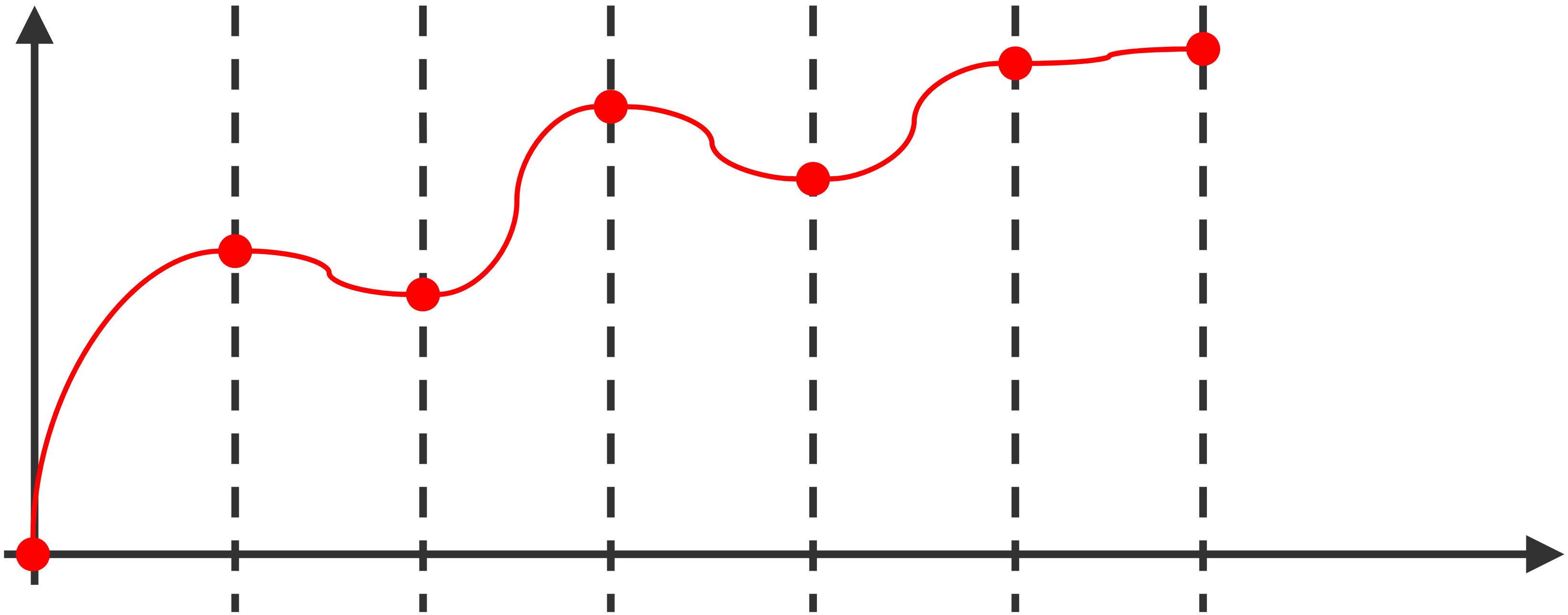


## Problem statement

Can we find?

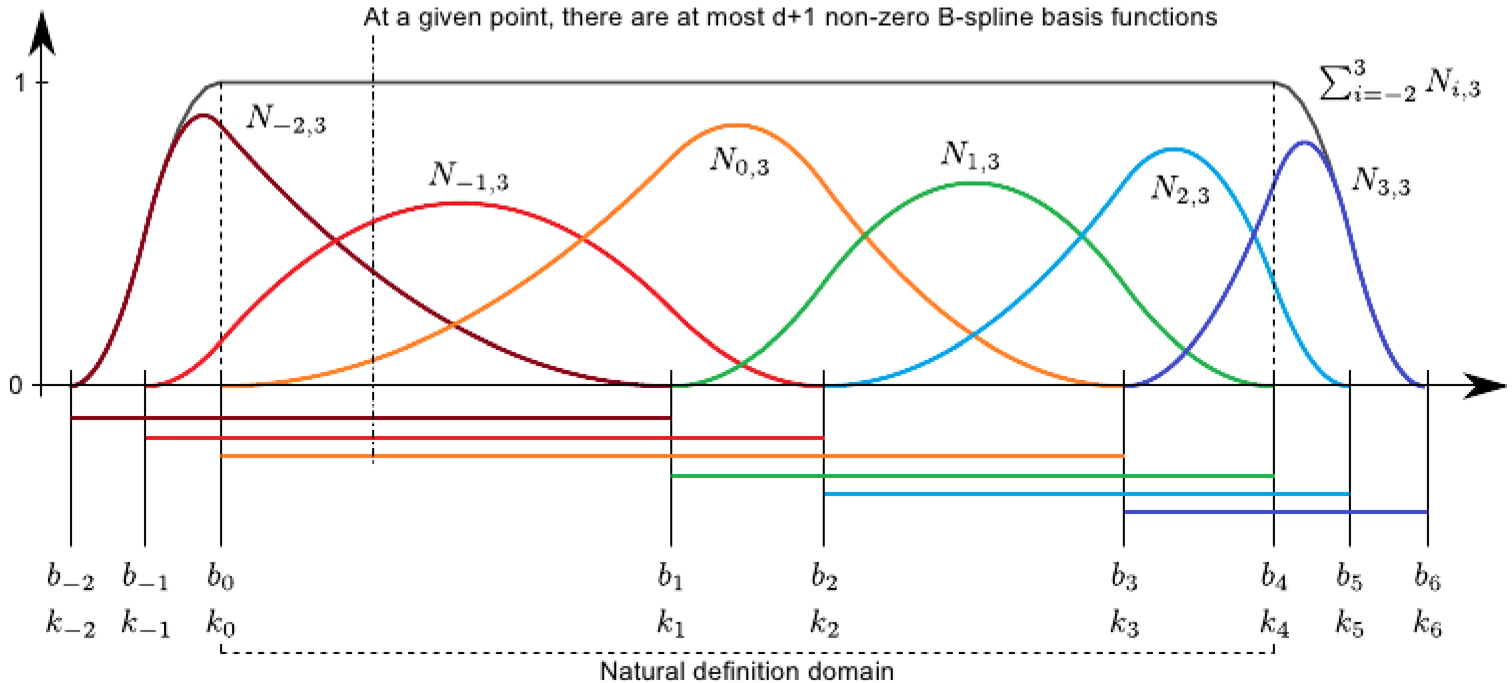
- A single kinetic rate law
- For all cases
- With a predetermined shape
- Based on experimental data

# Method: Splines



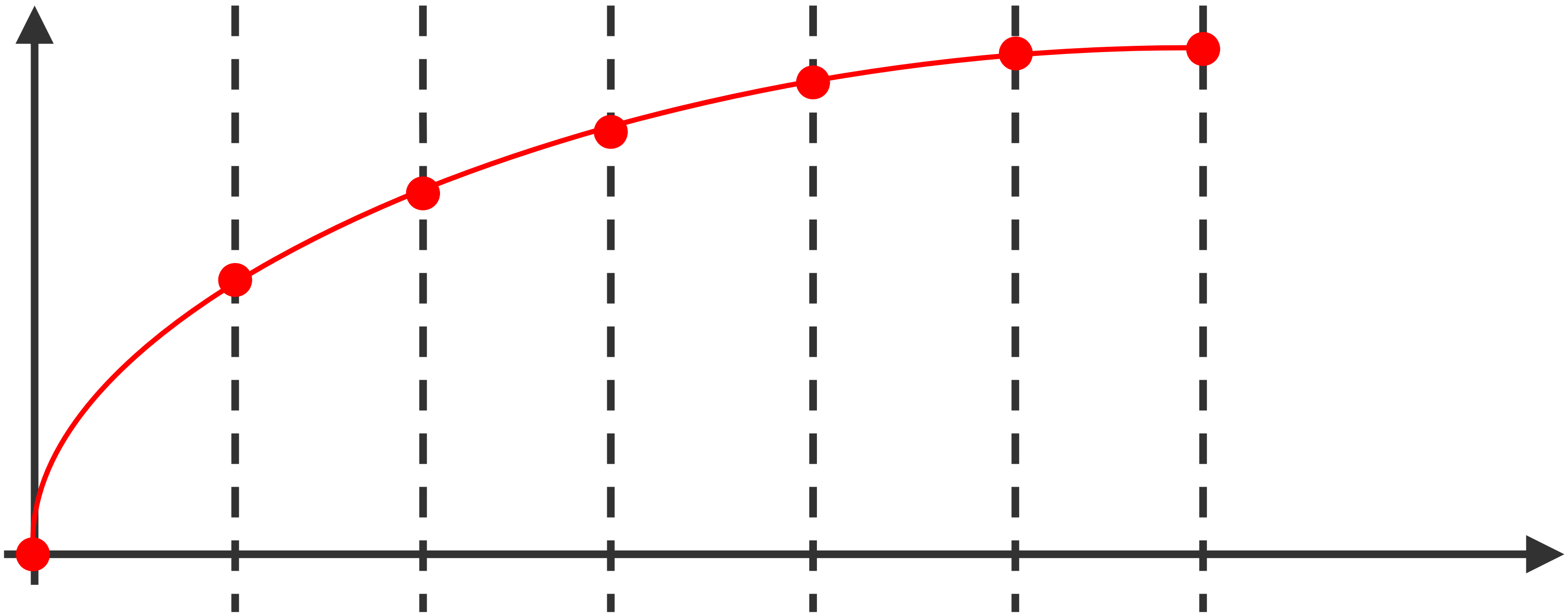
# Shape constrained spline (SCS) functions

Defined by the number and location of knots.




$$r_{SCS}(S) = \boldsymbol{b}(S)^T \cdot \theta$$

# Method: Shape Constrained Splines



# Method: Shape Constrained Splines

**Function**

Cubic spline

$$r_{SCS}(S) = b_0(S)^T \cdot \theta$$

Flexible
Semi-parametric
**Black-box**

**Shape constraints**

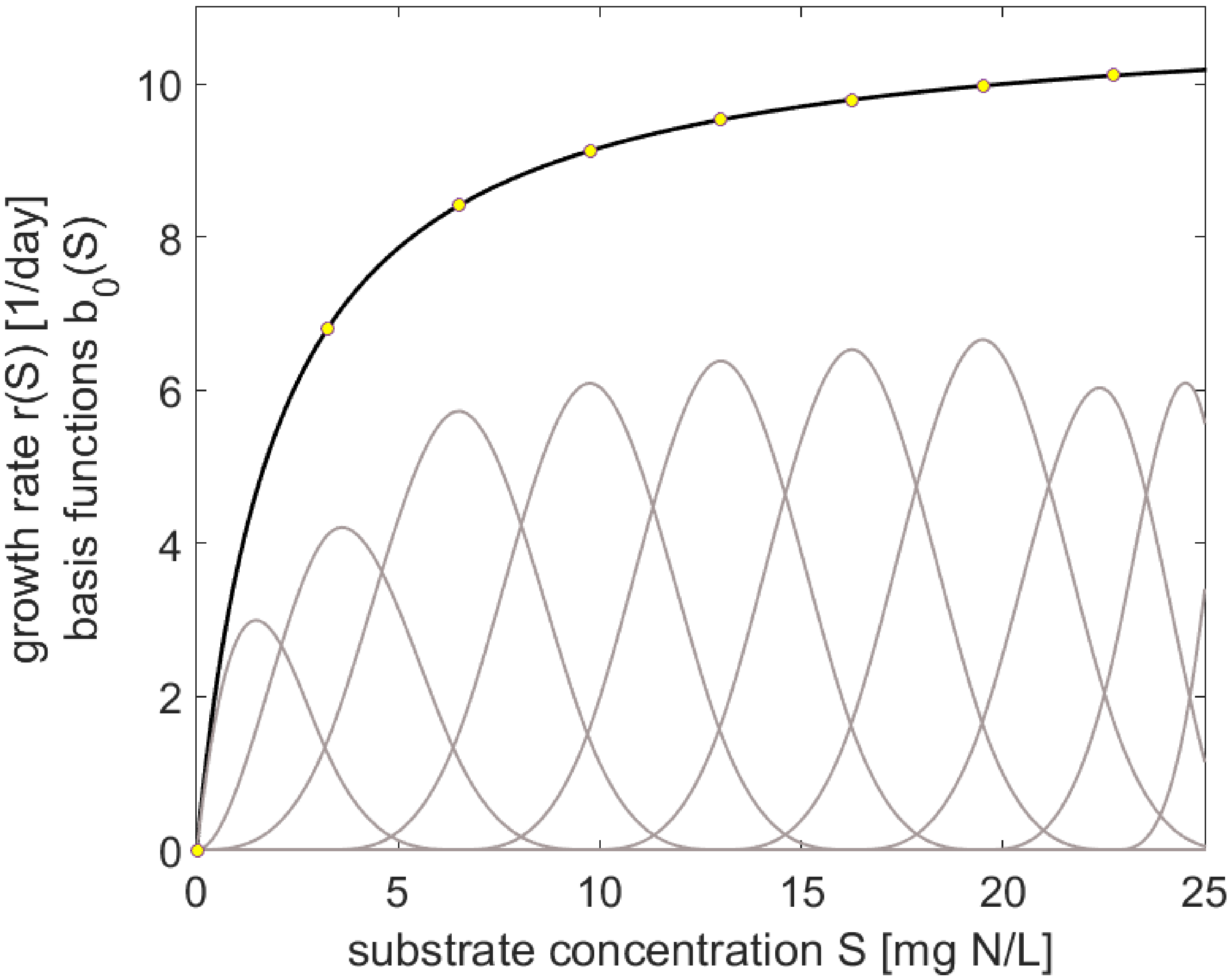
Often: linear in the parameters

Example: concave profile

$$b_2(S_k)^T \cdot \theta \leq 0 \qquad \forall\, k = 1, \dots, n_k$$

Prior knowledge
Smoothness
**White-box**

# Method: Shape Constrained Splines



# Method: what has changed?

## Previous work

$$\tilde{\boldsymbol{y}}(t) = f(t, \boldsymbol{\theta}) + e(t)$$

$$\boldsymbol{\theta} \in \boldsymbol{\Omega}$$

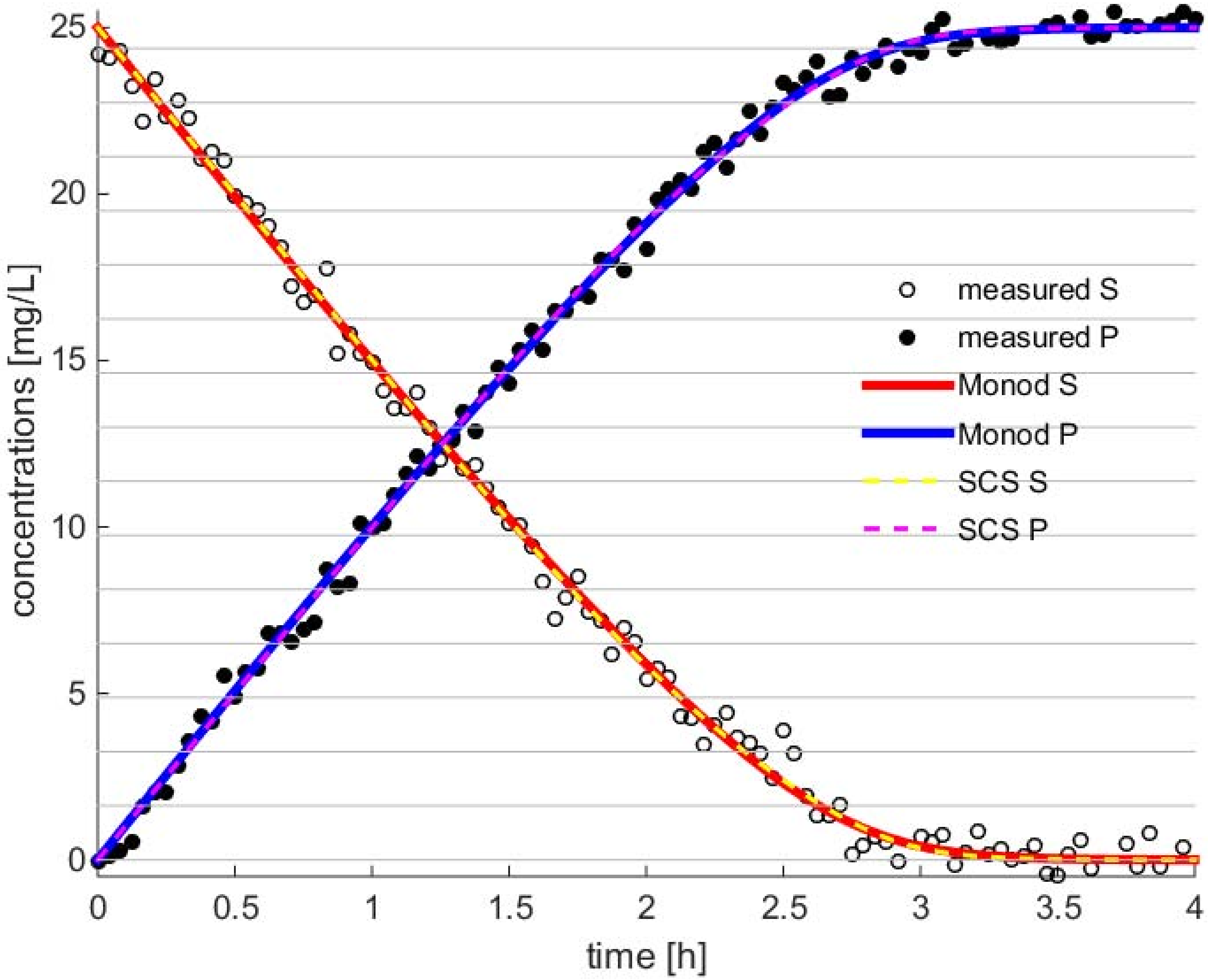
## Current work

$$\dot{x}(t) = -f(x(t), \boldsymbol{\theta}), \quad x(\mathbf{0}) = 0$$

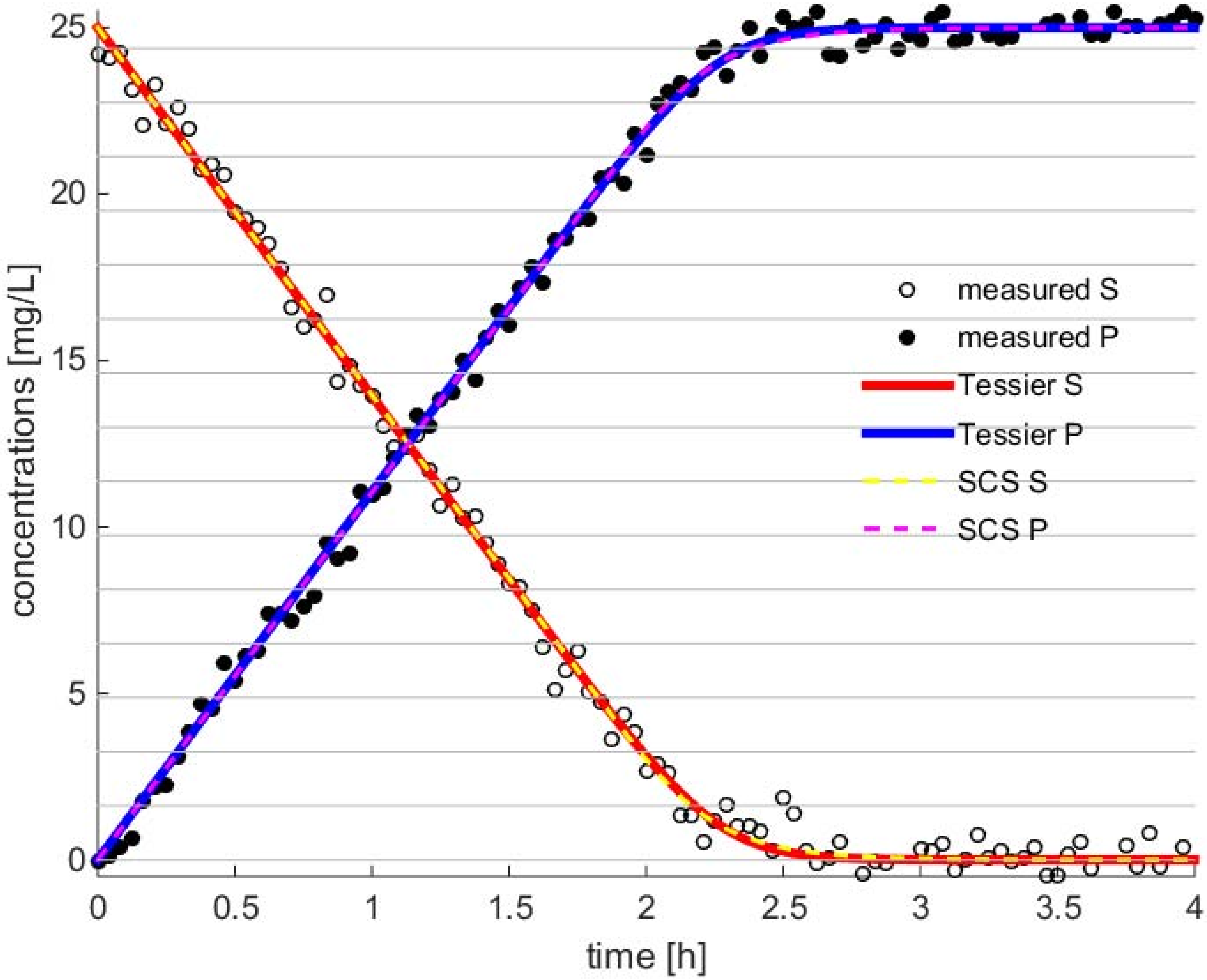
$$\tilde{\boldsymbol{y}}(t) = \boldsymbol{c}\, x(t) + \boldsymbol{d}\, e(t)$$

$$\boldsymbol{\theta} \in \boldsymbol{\Omega}$$

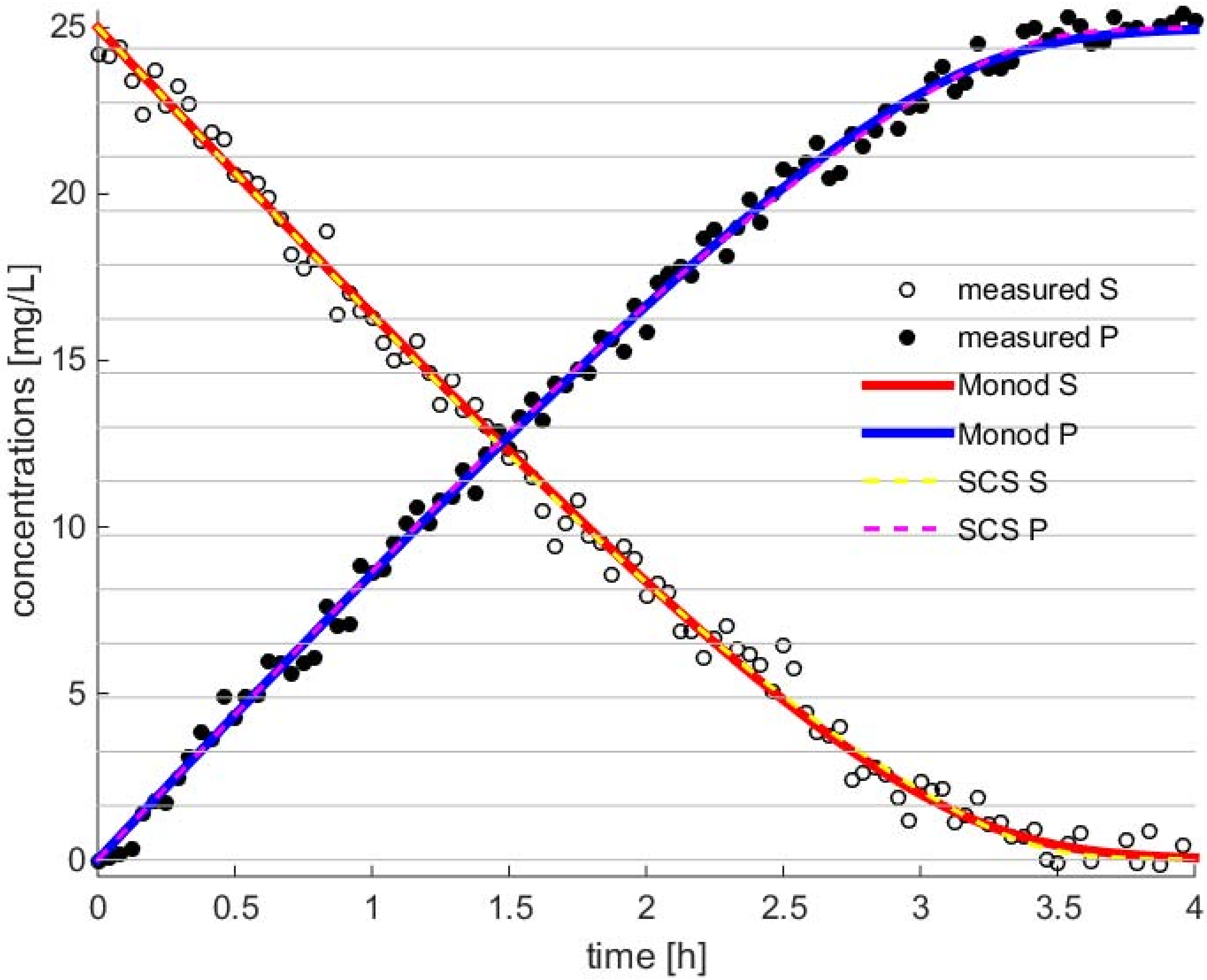
# Results: Monod



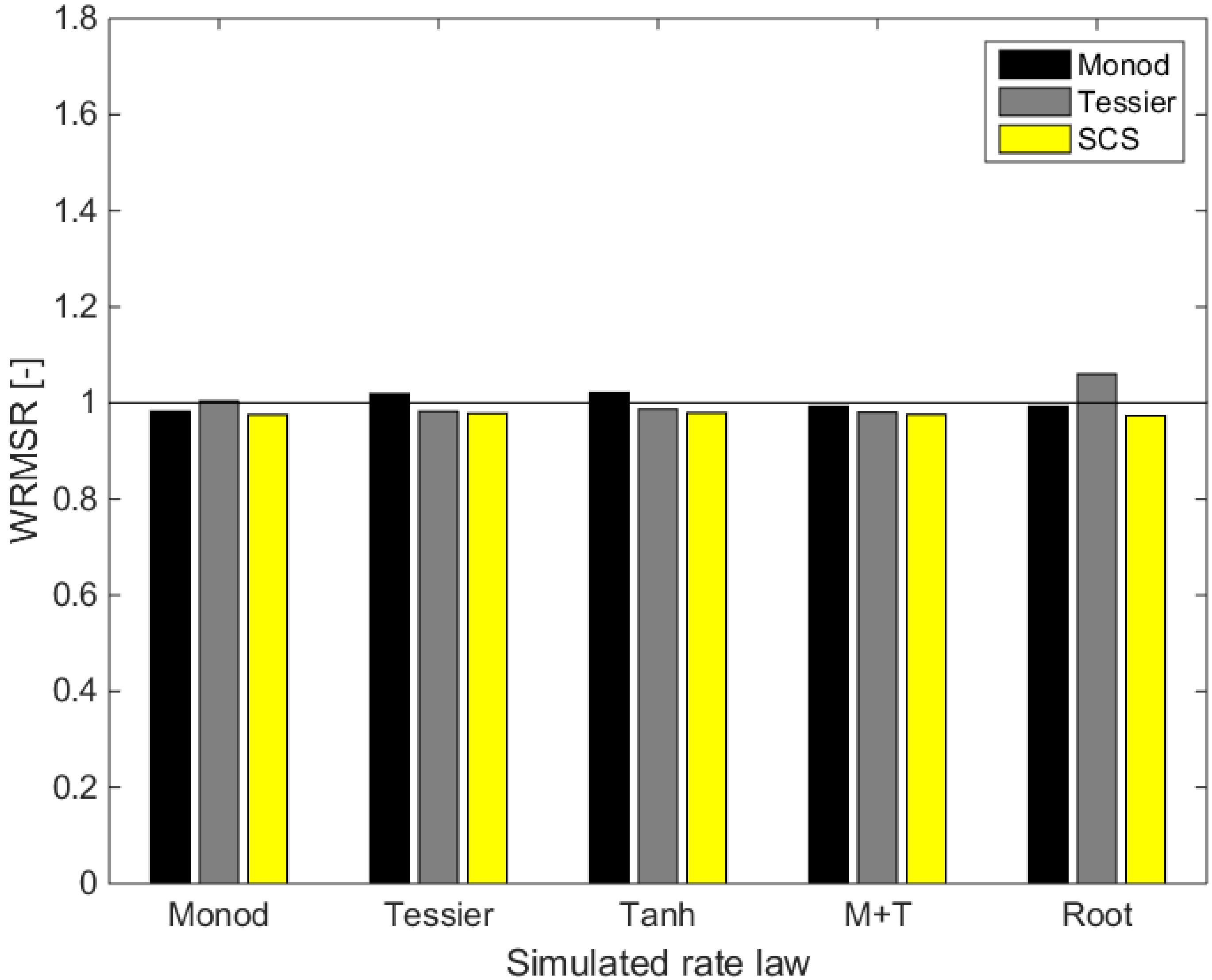
# Results: Tanh



## Results: Root



# Comparing all: WRMSR



# Conclusions / Perspectives

- **Shape constrained spline functions as rate models**
- **Near-universal property**
- **Advantages**
  - One-for-all model structure
  - Only one parameter optimization
- **Coming up**
  - Different shape (ecoSTP2016)
  - Laboratory experiment
  - Uncertainty analysis
  - Increased complexity

## Summary

We found

- A single kinetic rate law
- For all (substrate affinity) cases
- With a predetermined shape
- Based on (simulated) experimental data

## Different shape