

# Biokinetic process model diagnosis with shape-constrained spline functions

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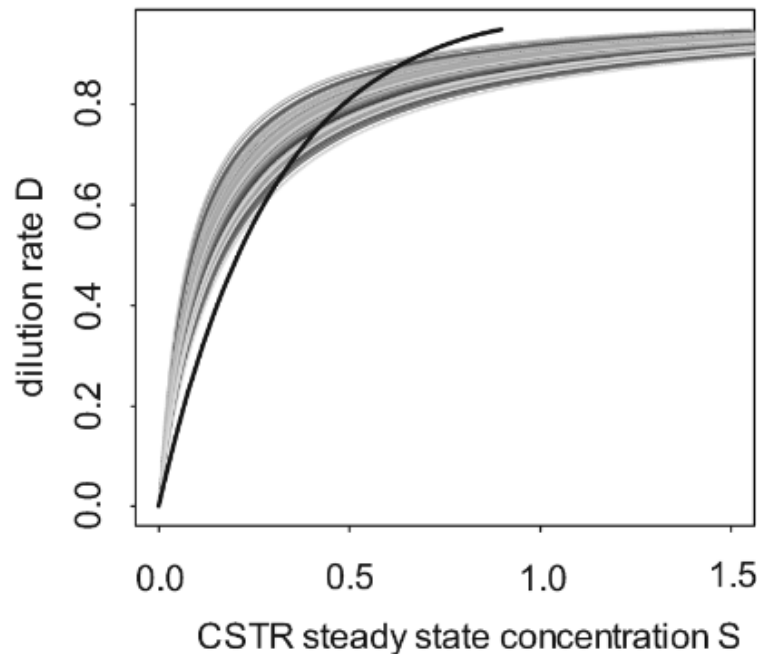
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## Setting the stage

- Biological wastewater treatment (e.g. nitrification)
- Mathematical models = helpful tools
- Biokinetic process models (e.g. ASM) well established
- Express bacterial growth rates with respect to concentration of substrate
- Examples: Monod and Tessier kinetics

# Problem

- Bacteria unlikely to follow idealized kinetics
- Typically, Monod = default
- Inappropriate/wrong model can lead to errors
  - design and optimization purposes



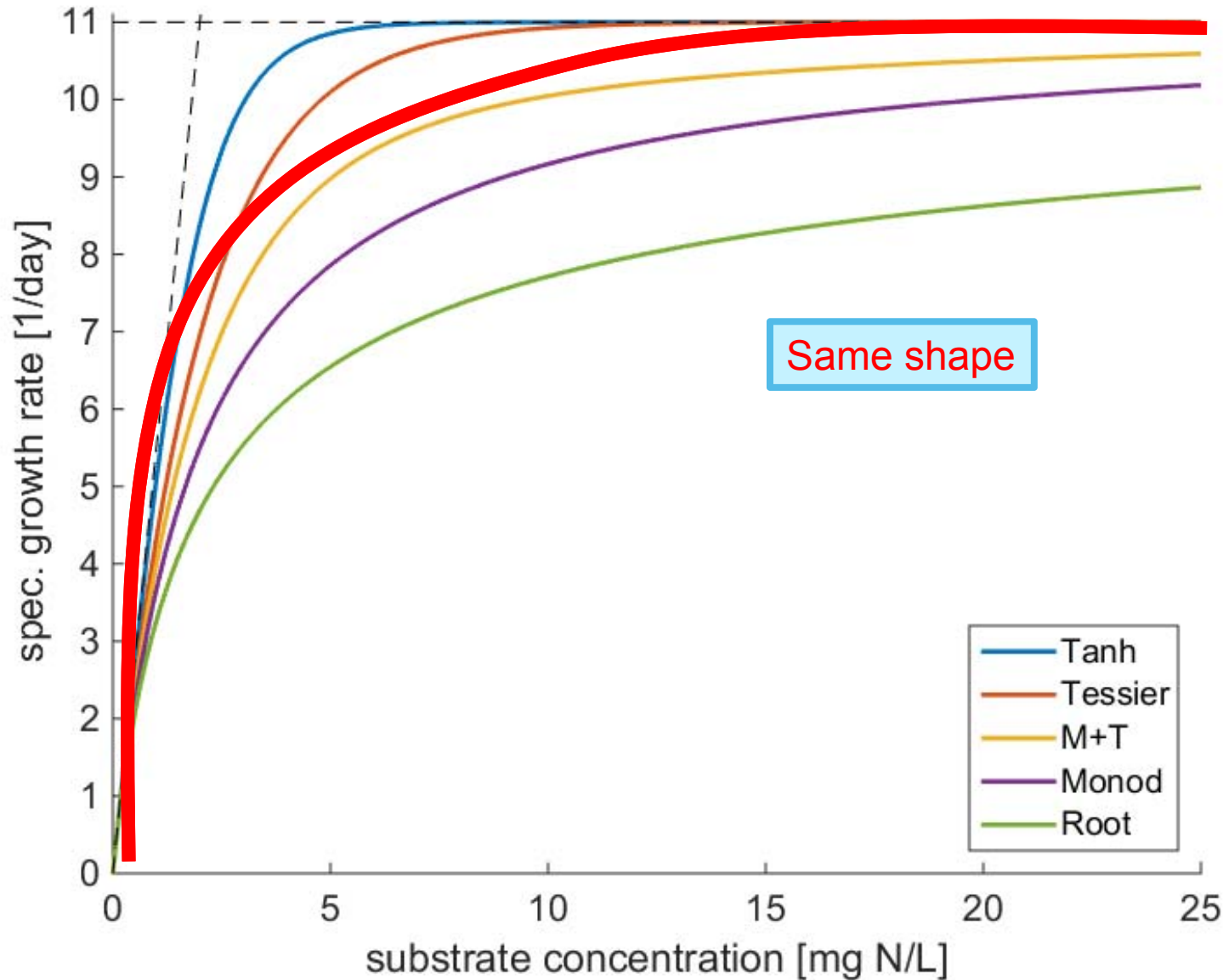
**FIGURE 4.** Prediction for CSTR steady state concentrations  $S$  across all dilution rates  $D$  for  $\sigma = 0.1$ ;  $K_S^{\text{Tessier}} = 0.3$ . 1000 MC simulations for Monod model and prediction with true Tessier model (solid black line).

Neumann & Gujer (2008)  
Underestimation of uncertainty  
in statistical regression of  
environmental models:  
Influence of model structure  
uncertainty, *Environ. Sci.  
Technol.* 42: 4037-4043.

# Justification

- Convenient to use the same model
- Monod is very simple, 2 parameters
- Investigating the structure takes time
- Library of candidate models is never exhaustive
- No guarantee that results will be improved much

# Kinetic growth rates



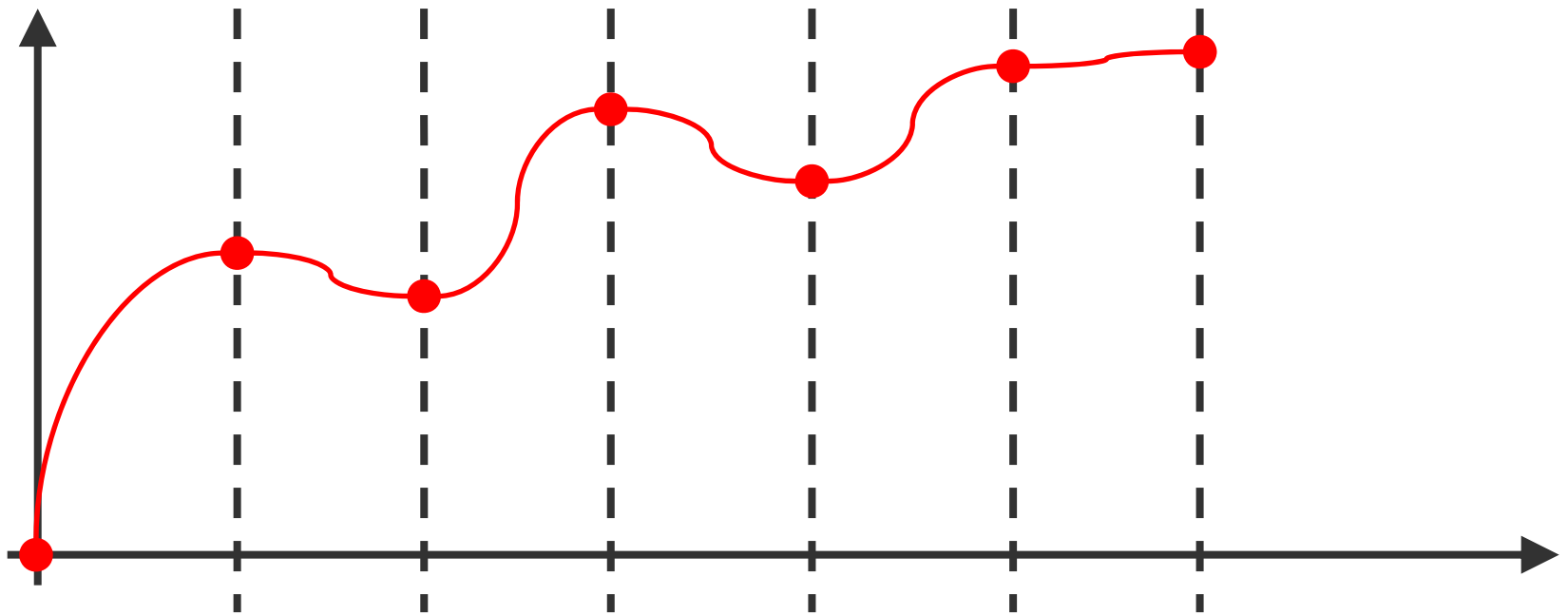
# Problem statement

Can we find?

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

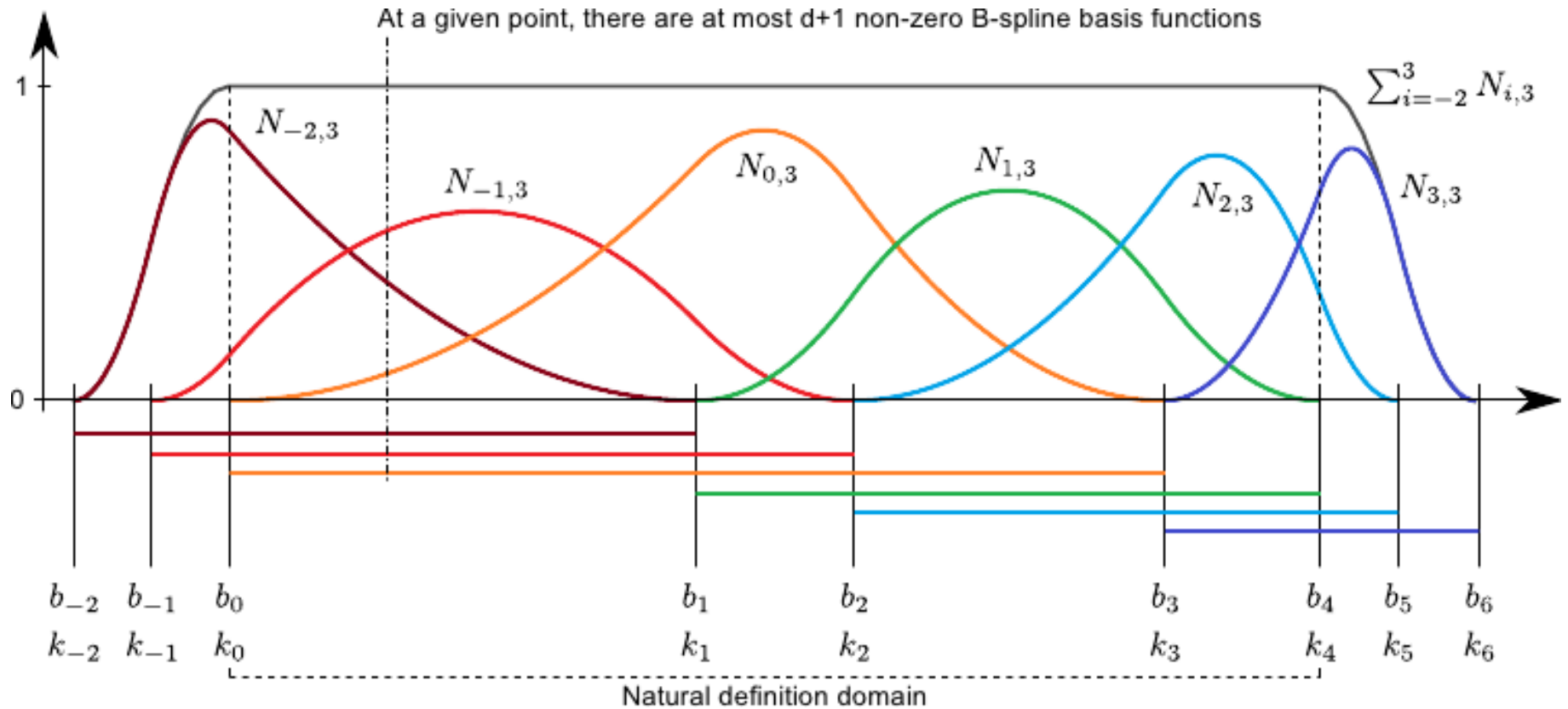
# Spline functions

Defined by the number and location of knots.



# Spline functions

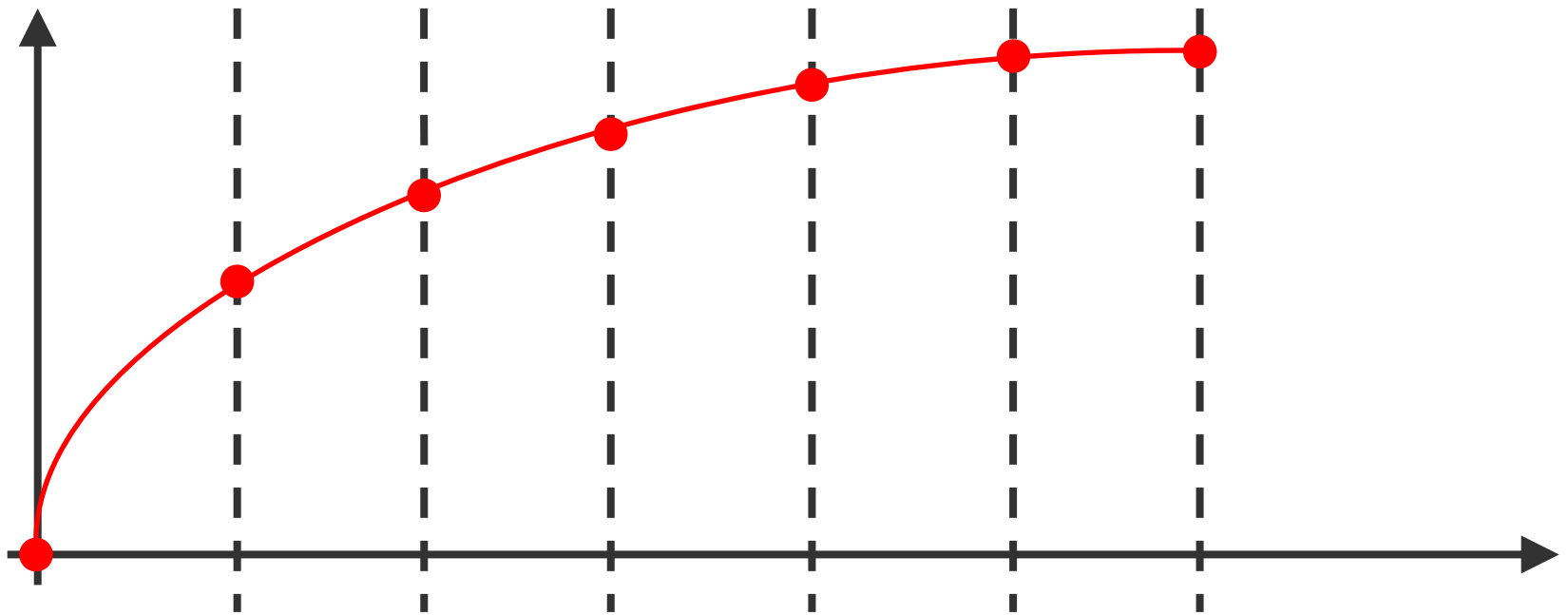
Defined by the number and location of knots.



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



# Shape constrained spline (SCS) functions



# Shape constrained spline (SCS) functions

- **Function**
- Cubic spline

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

Flexible  
Semi-parametric  
**Black-box**

## Shape constraints

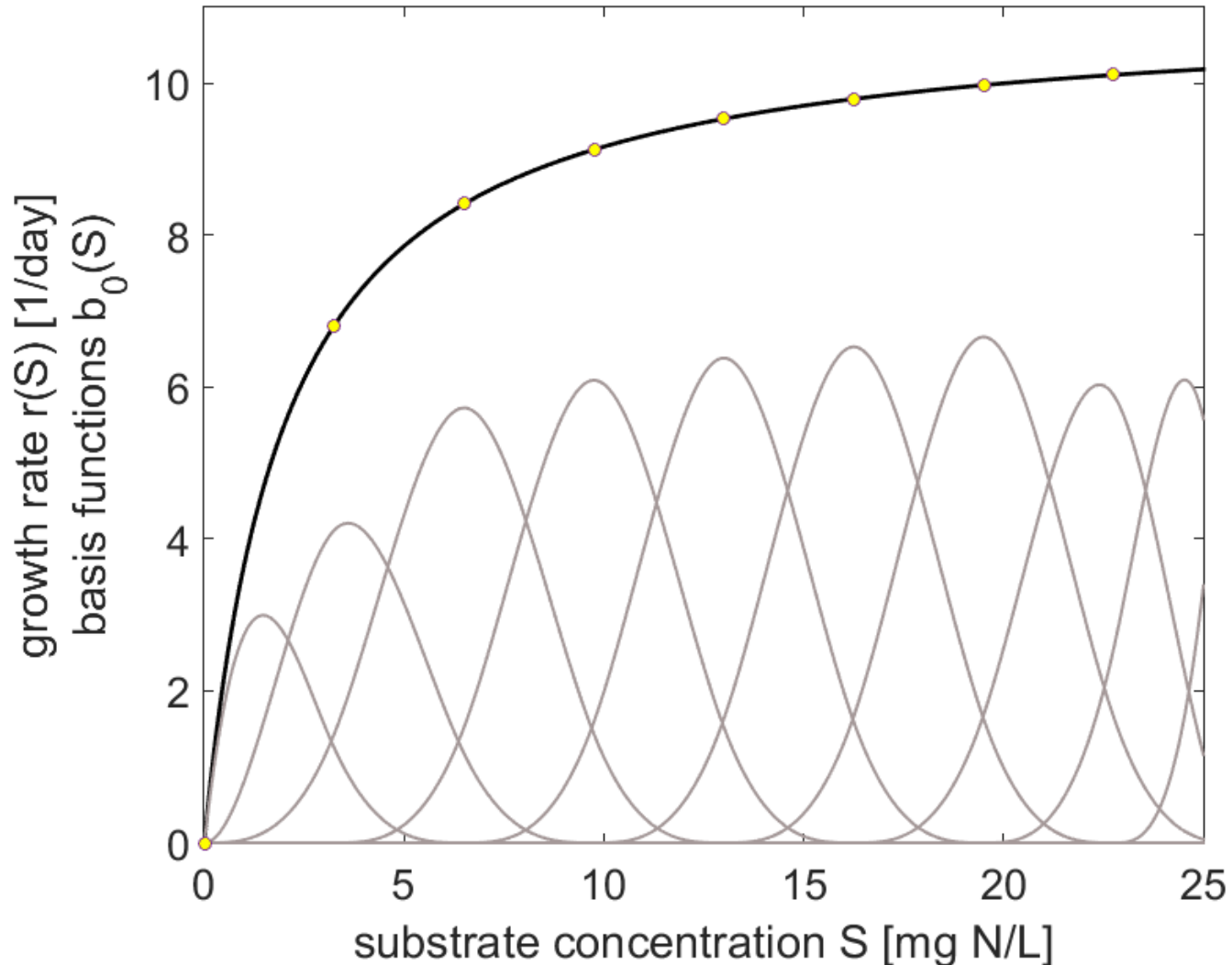
Often: linear in the parameters  
Example: concave profile

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

Prior knowledge  
Smoothness  
**White-box**

# Shape constrained spline (SCS) functions

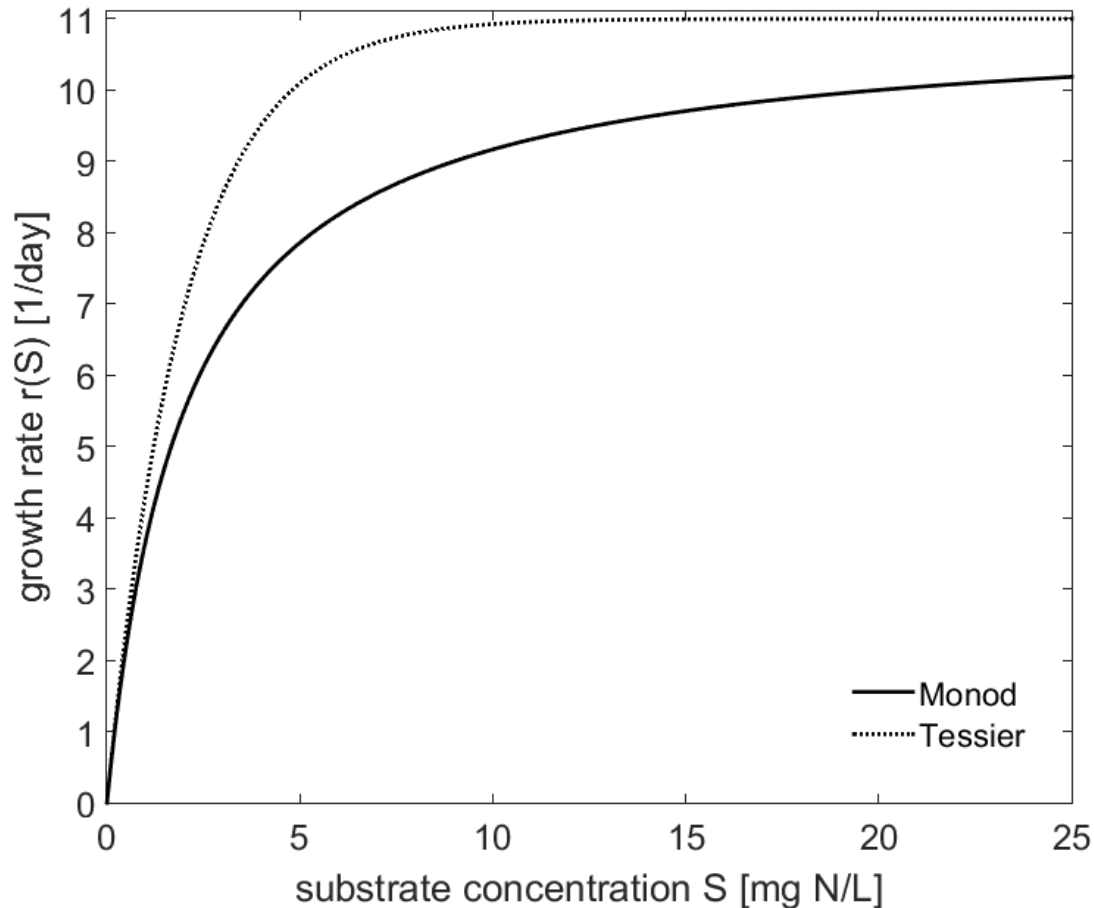
Shape: concave, monotonically increasing. 9 knots.



# Library of candidate models

- Most common (non-inhibited): Monod and Tessier

$$r_{MONOD}(S) = a^{max} \frac{S}{S + K_S} \quad r_{TESSIER}(S) = a^{max} (1 - e^{-S/K_S})$$



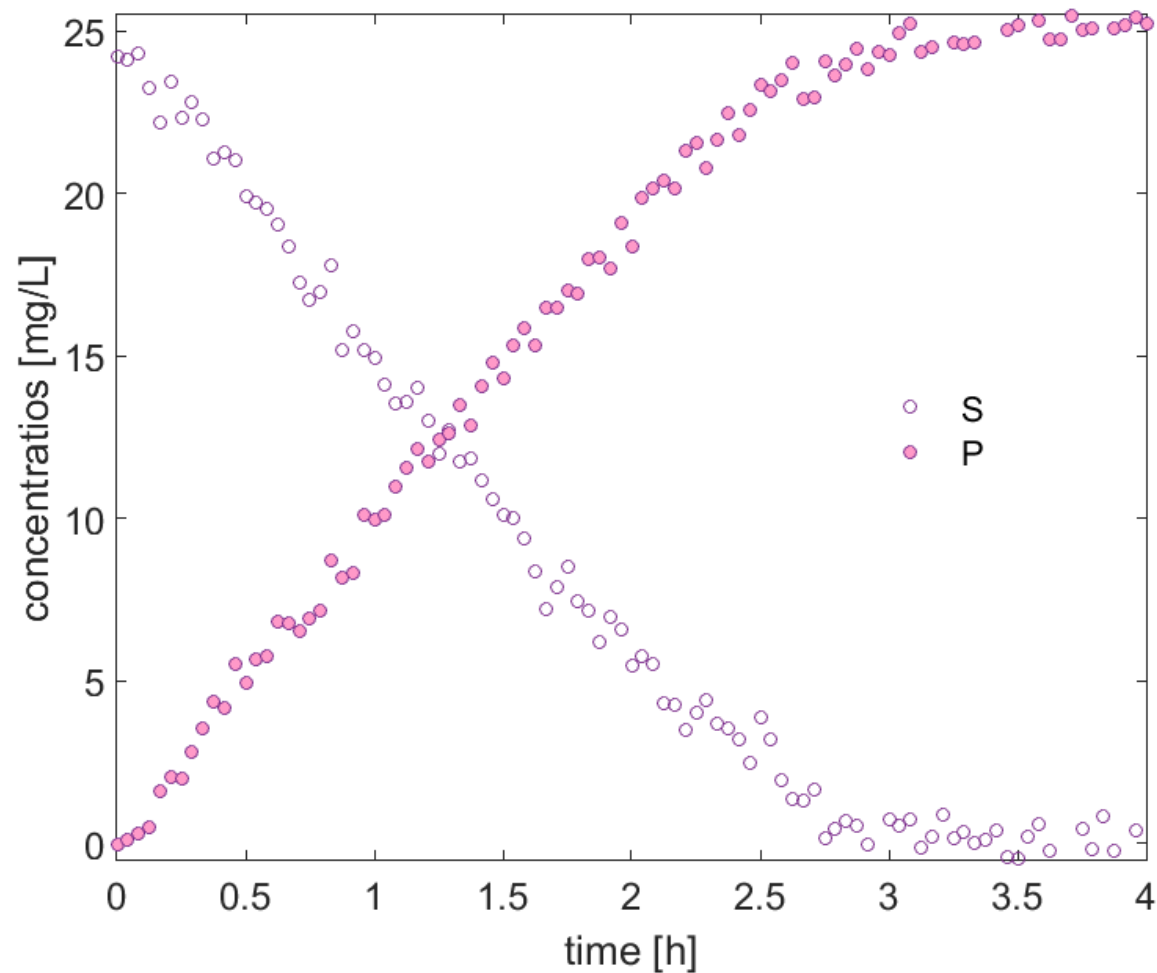
# Methods

- Numerical approach
  - simulate noisy concentration data from a batch reactor
  - simple kinetic model
  - assumptions: negligible bacterial growth
  - fit parameters of library models and of SCS model
  - use WRMSR as measure
- Matlab
  - use of Functional Data Analysis toolbox

# Simulation with Monod

$$\frac{dS}{dt} = -r(S), \quad S(0) = S^0$$

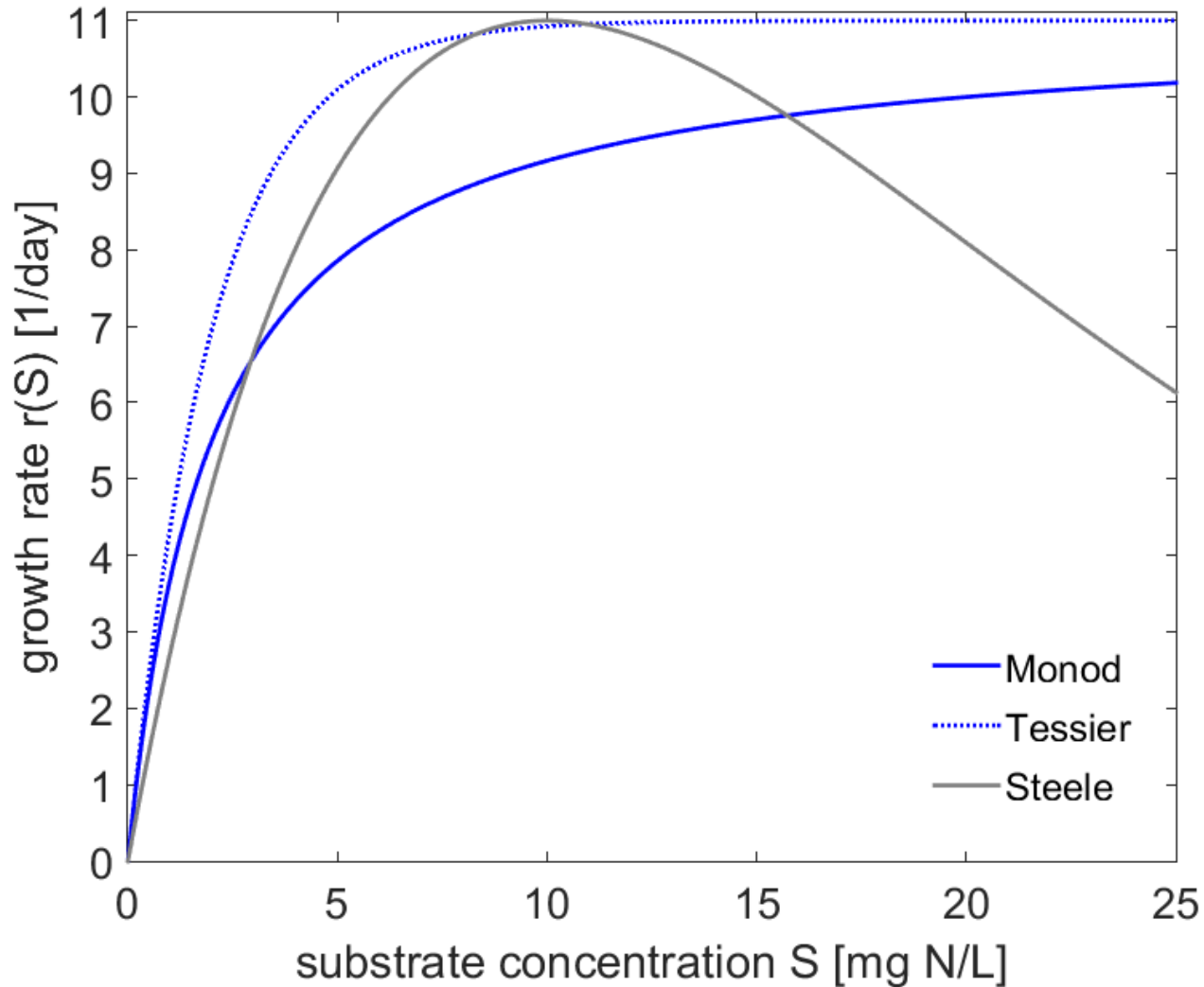
$$P(t) = S^0 - S(t)$$



# Scenario

- Measurements available
- Aim: identify structure of biokinetic model
- Approach:
  - use SCS to determine shape
  - limit the search in a library of conventional models

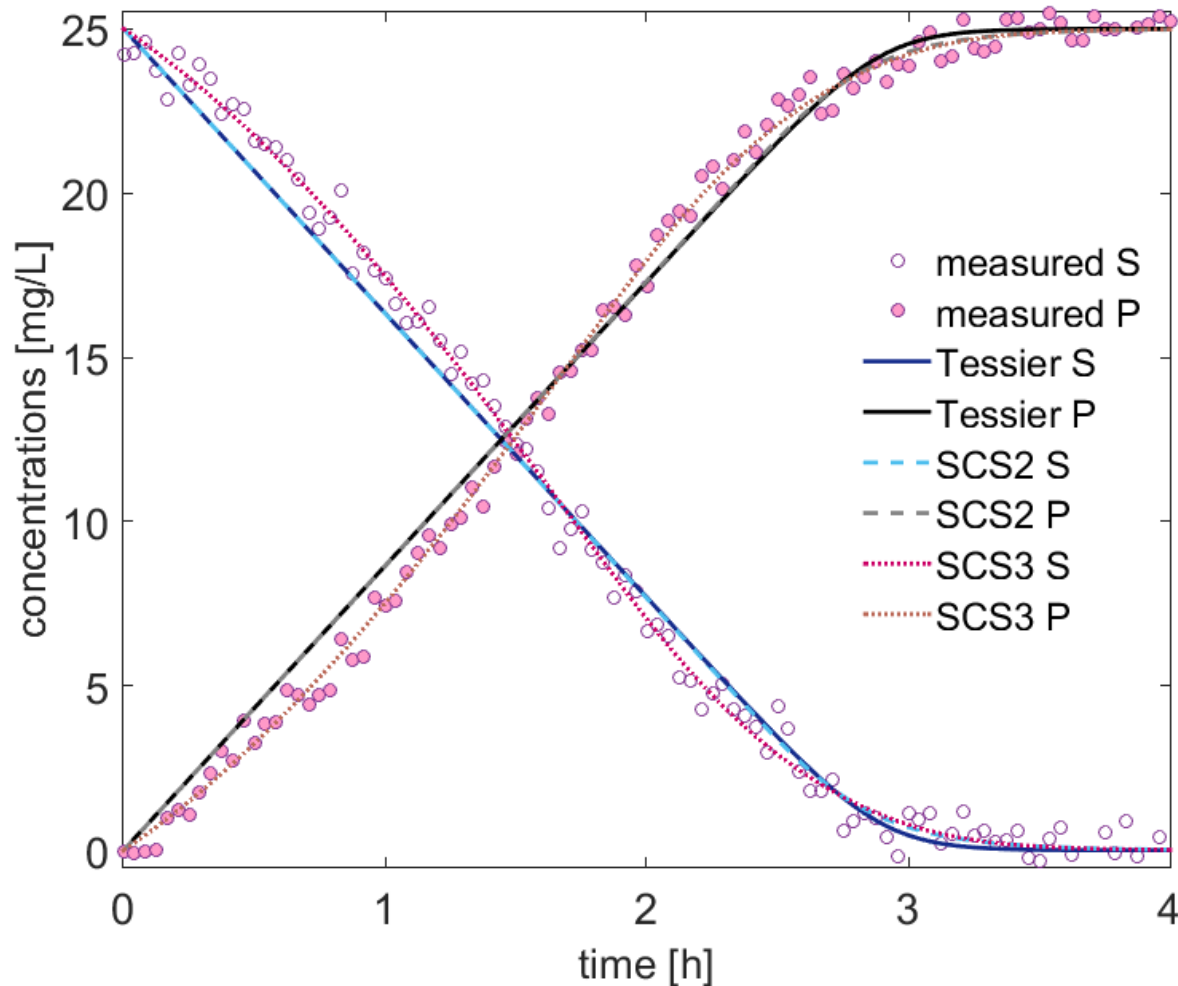
# Scenario – simulated rate laws



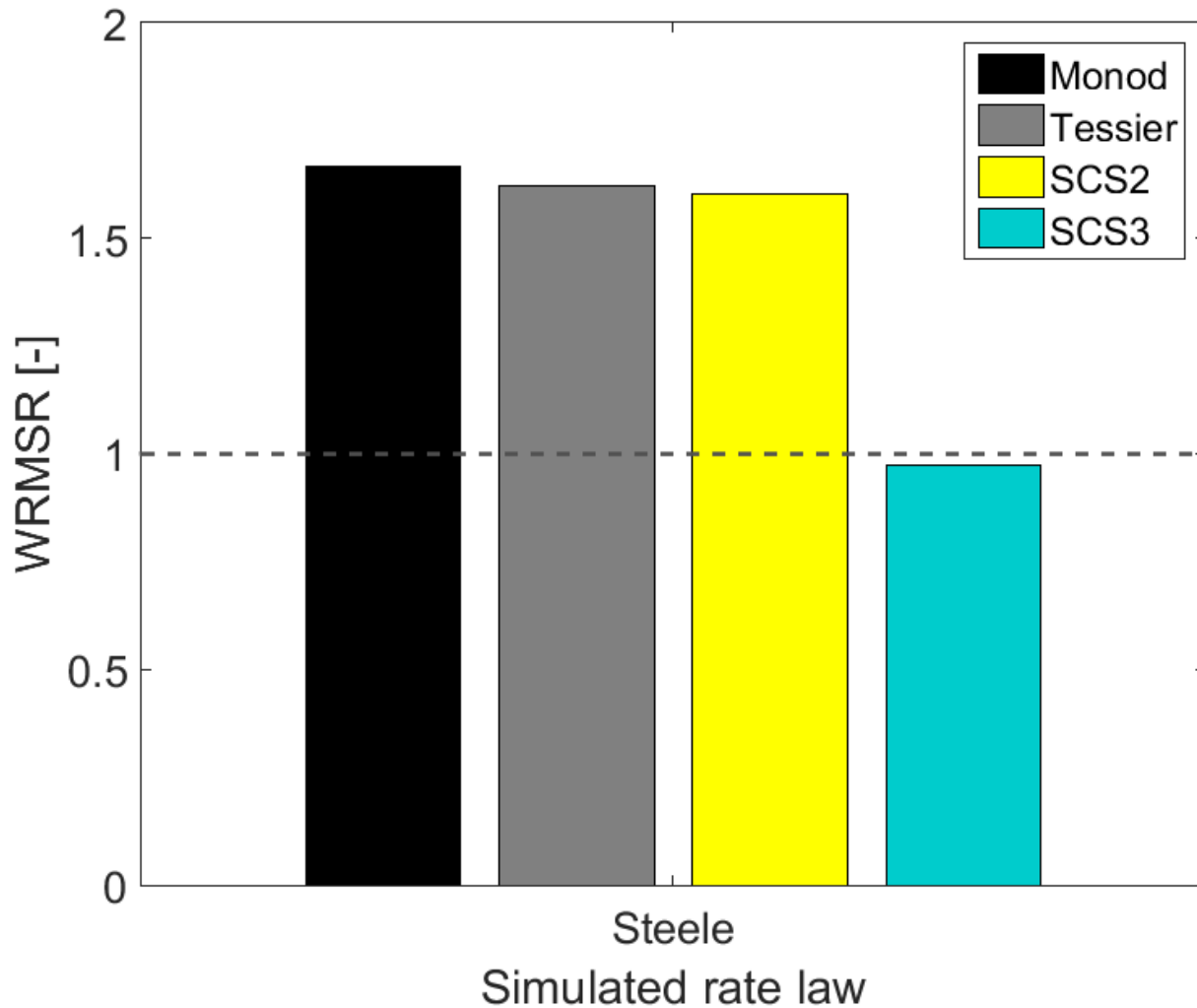


# Results

Use library models (Monod, Tessier) and different SCS models to fit measurement data (Steele)



# Results - WRMSR



SCS2 = concave,  
monotonically  
increasing

SCS3 = concave

# Conclusions

- Shape-constrained spline functions successfully used to diagnose shape of biokinetic model
- Easier and quicker diagnosis and identification of model shape
- Helpful when underlying rate law unknown and a potentially wrong model is used

# Shape constrained spline (SCS) functions

## Benefits of SCS:

- Representing a wide range of known behaviors – one function
- Optimization of one parameter set only instead of multiple sets
- Easier to update

## Future work

- Several different shapes and a variety of different scenarios
- Real measurement data
- More complex models/scenarios
- Uncertainty analysis

Thank you for your attention!