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Eawag:
Swiss Federal Institute of Aquatic
Science and Technology

eawag
aquatic research

Modelling Aquatic Ecosystems
Course 701-0426-00

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Eawag, Swiss Federal Institute of Aquatic Science and Technology

Structure of the Course

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1. Introduction, principles of modelling environmental systems, mass balance in a mixed reactor, process table notation, simple lake plankton model
   Exercise: R, `ecosim`-package, simple lake plankton model
   Exercise: lake phytoplankton-zooplankton model
2. Process stoichiometry Exercises: analytical solution, calculation with `stoichcalc`
3. Biological processes in lakes
4. Physical processes in lakes, mass balance in multi-box and continuous systems Exercise: structured, biogeochemical-ecological lake model
   Assignments: build your own model by implementing model extensions
5. Physical processes in in rivers, bacterial growth, river model for benthic populations Exercise: river model for benthic populations, nutrients and oxygen
6. Stochasticity, uncertainty, Parameter estimation
   Exercise: uncertainty, stochasticity
7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback

Goals

- Review exercise 2 and clarify open questions
- Acquire knowledge in process stoichiometry to bridge between ecological and biogeochemical processes.
- Learn to calculate stoichiometric coefficients
  from chemical substance notation (chapter 4.3.1)
  and parameterized elemental mass fractions (chapter 4.3.2).

Review Exercise 2: Model description

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chapter 11.2

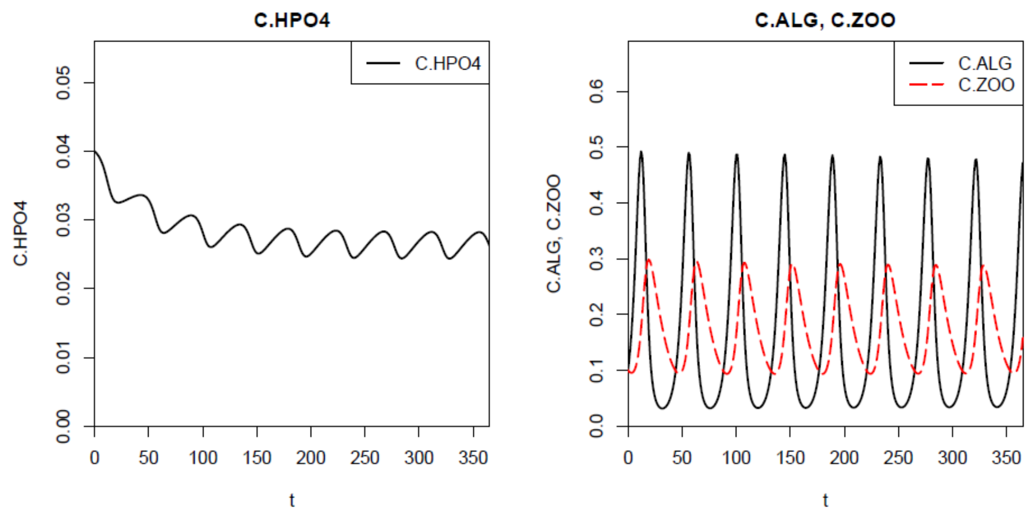
Process	Substances / Organisms HPO4 $[gP/m^3]$	ALG $[gDM/m^3]$	ZOO $[gDM/m^3]$	Rate
Growth of algae	$-\alpha_{P,ALG}$	1		$\rho_{gro,ALG}$
Death of algae		-1		$\rho_{death,ALG}$
Growth of zooplankton		$-\frac{1}{Y_{ZOO}}$	1	$\rho_{gro,ZOO}$
Death of zooplankton			-1	$\rho_{death,ZOO}$

here units of the state variables in the model

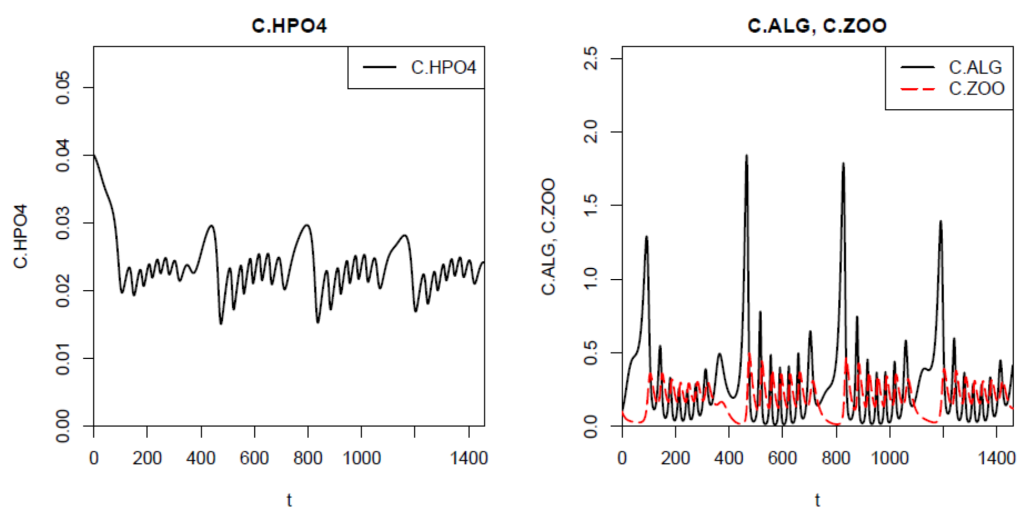
Rate	Rate expression
$\rho_{gro,ALG}$	$k_{gro,ALG,T_0} \cdot \exp\Big(\beta_{ALG}(T - T_0)\Big) \cdot \frac{1}{\lambda h} \log\left(\frac{K_I + I_0}{K_I + I_0 \exp(-\lambda h)}\right) \cdot \frac{C_{HPO_4^{2-}}}{K_{HPO_4^{2-},ALG} + C_{HPO_4^{2-}}} \cdot C_{ALG}$
$\rho_{death,ALG}$	$k_{death,ALG}\, C_{ALG}$
$\rho_{gro,ZOO}$	$k_{gro,ZOO,T_0} \cdot \exp\Big(\beta_{ZOO}(T - T_0)\Big) \cdot C_{ALG}\, C_{ZOO}$
$\rho_{death,ZOO}$	$k_{death,ZOO}\, C_{ZOO}$

Review Exercise 2: Model results

Results for constant environmental conditions



Results for periodic environmental conditions



Review Exercise 2: Questions

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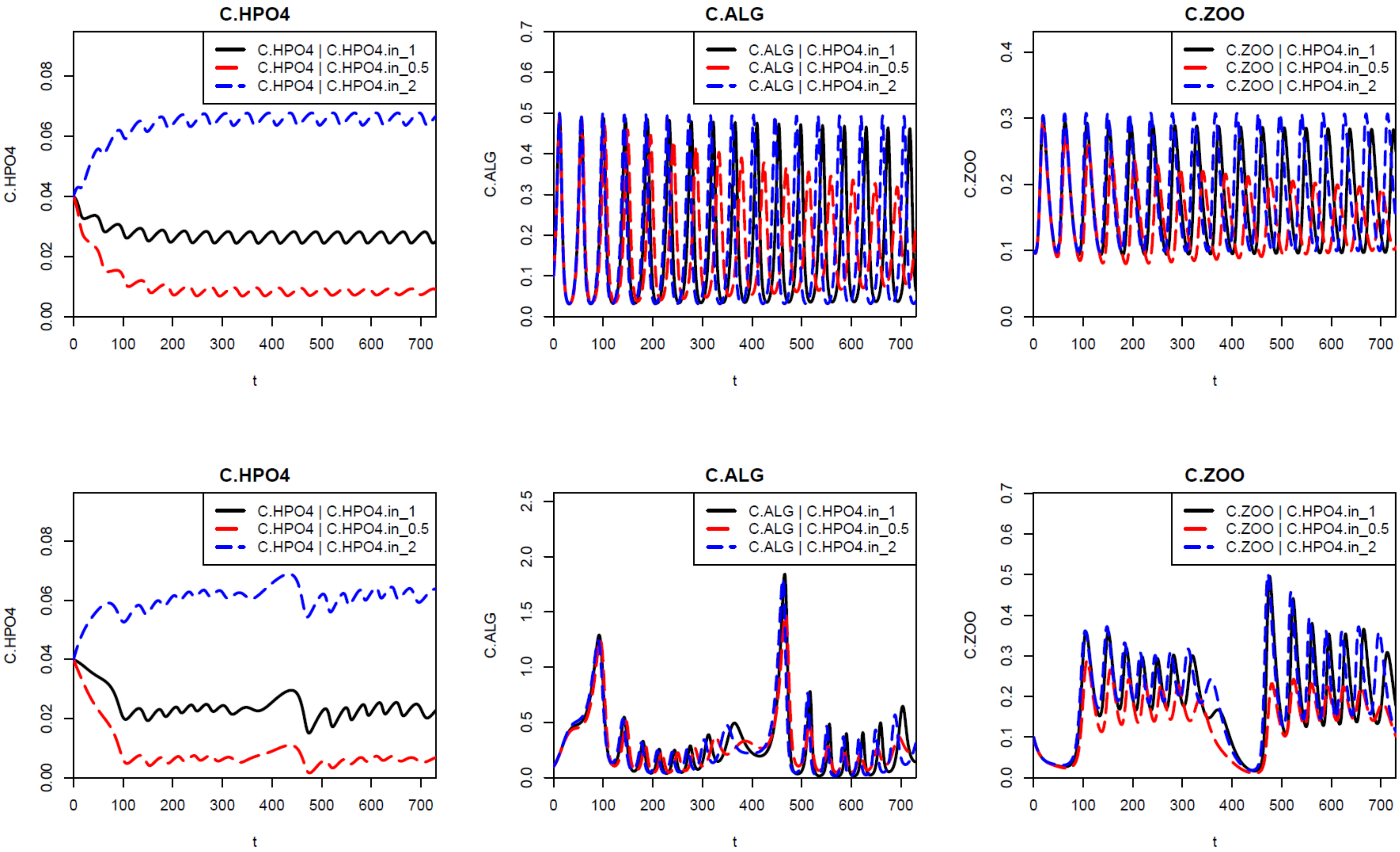
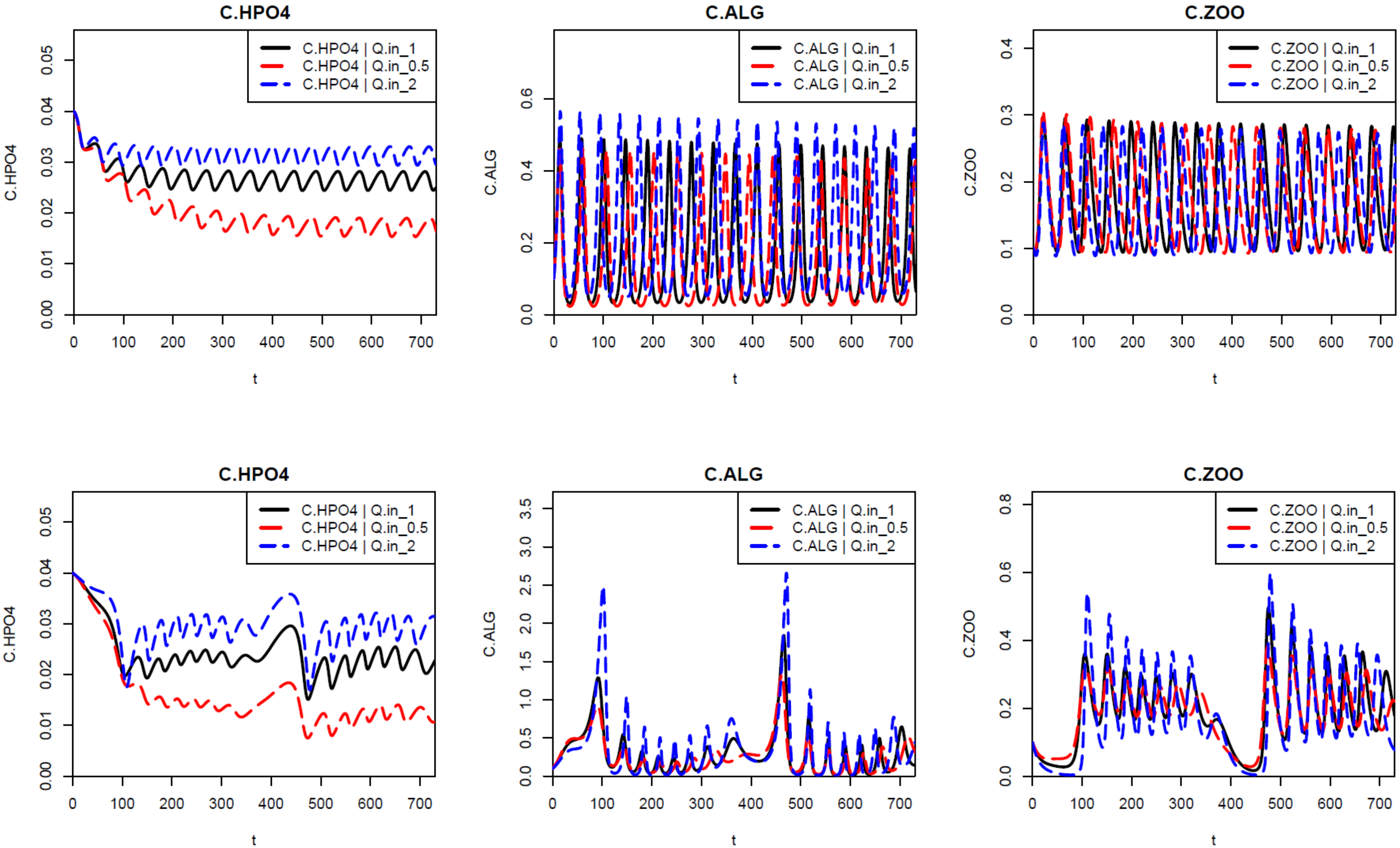
1. Are the algae concentrations controlled bottom-up (by phosphate limitation) or top-down (by grazing of zooplankton)?
2. What is the reason for oscillating concentrations under constant driving forces? What happens when you introduce periodic driving forces?
3. What are the main deficits of the model compared to a real lake?
4. What is your expectation regarding the response of the model to the change in each parameter, does the result match your expectation and can you explain the observed changes?

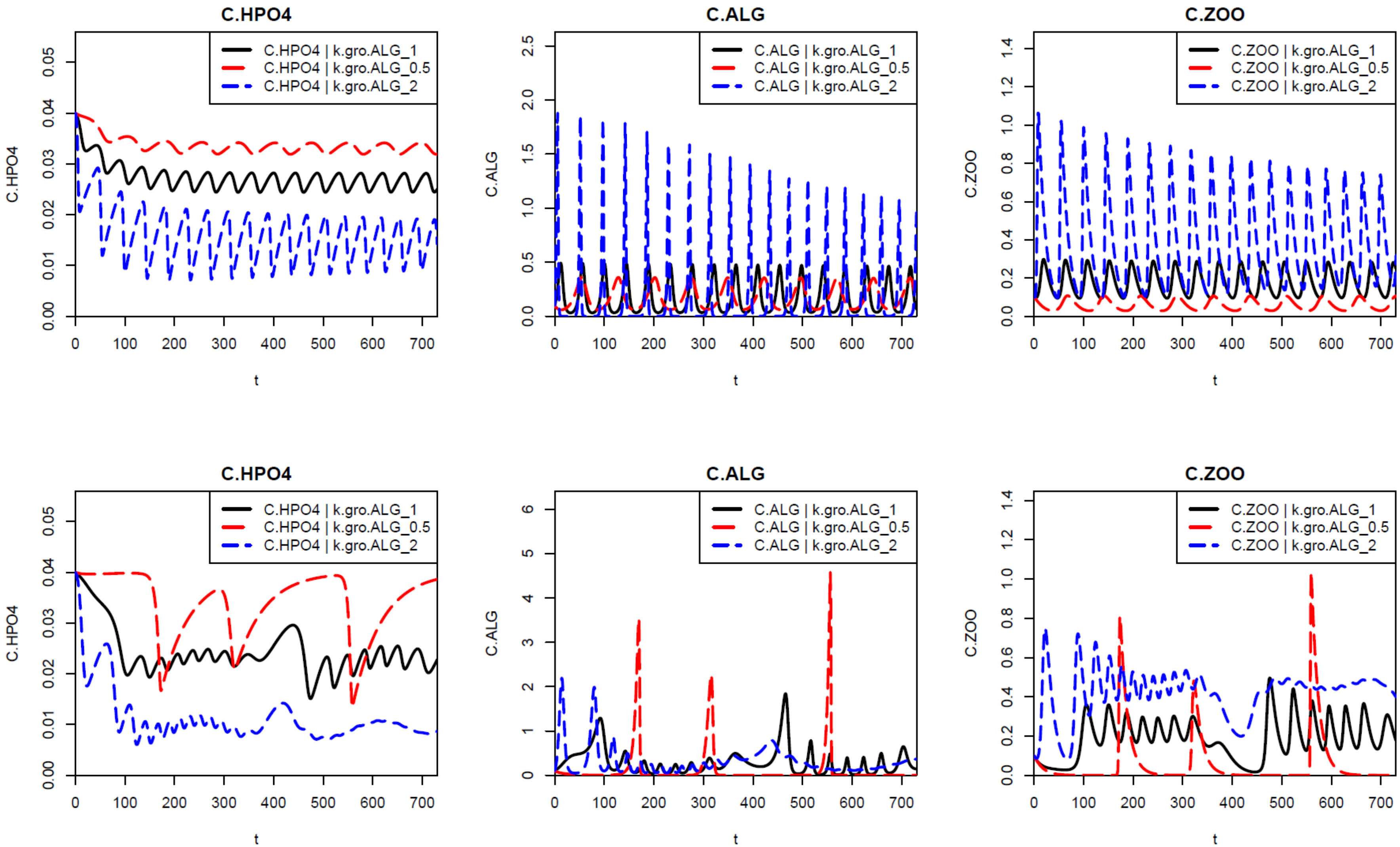
Review Exercise 2: Sensitivity Analysis



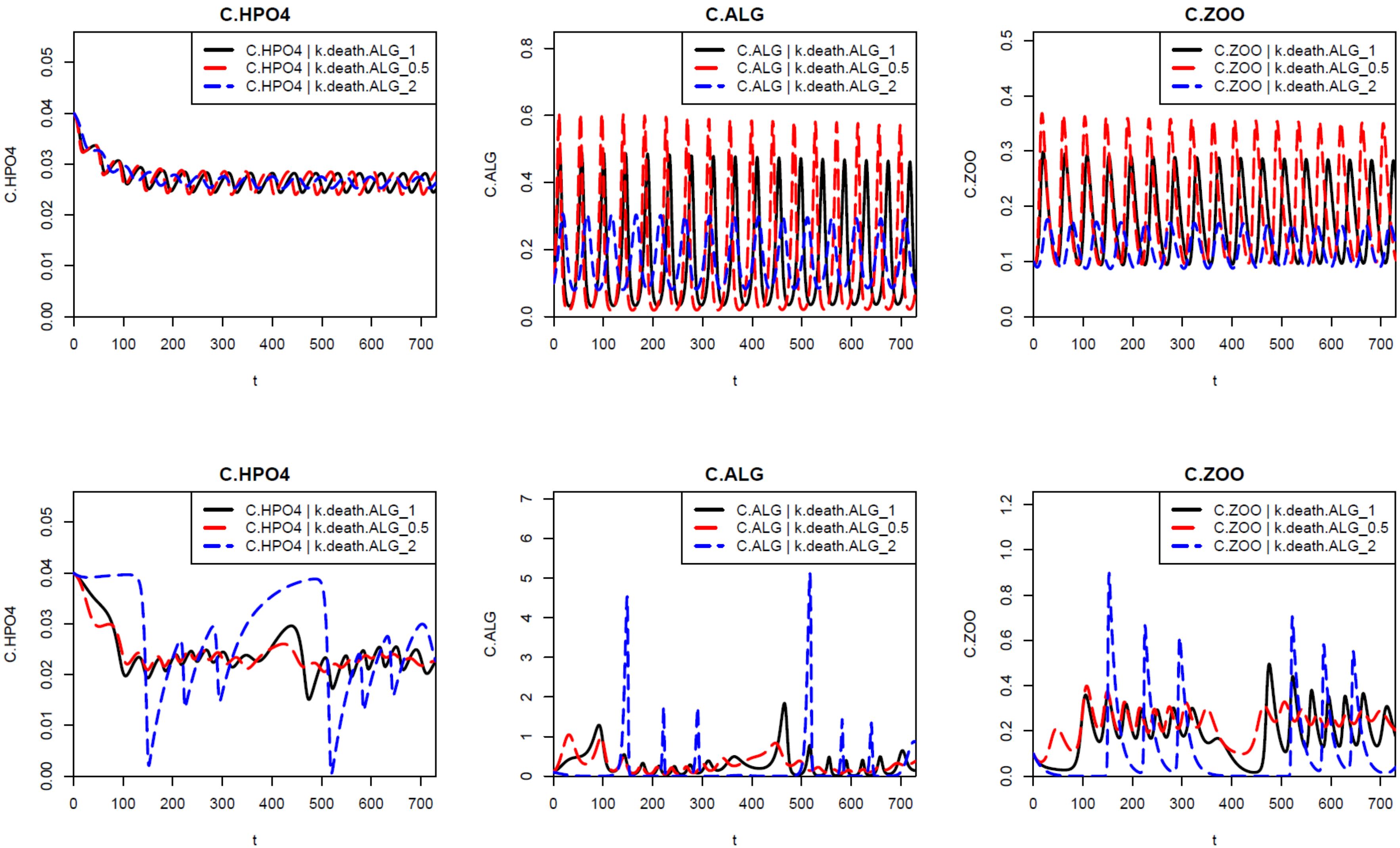
Review Exercise 2: Sensitivity Analysis



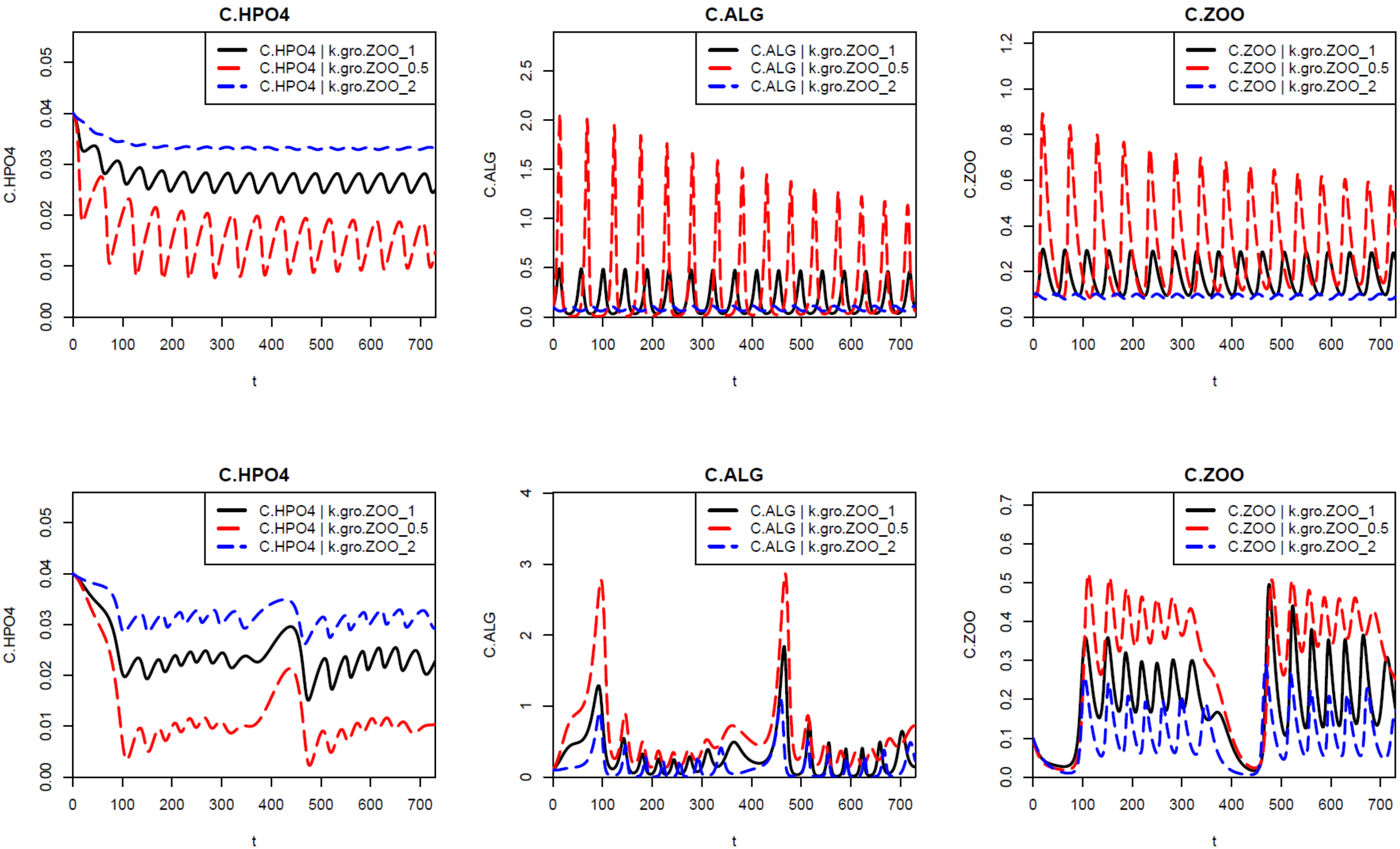
Review Exercise 2: Sensitivity Analysis



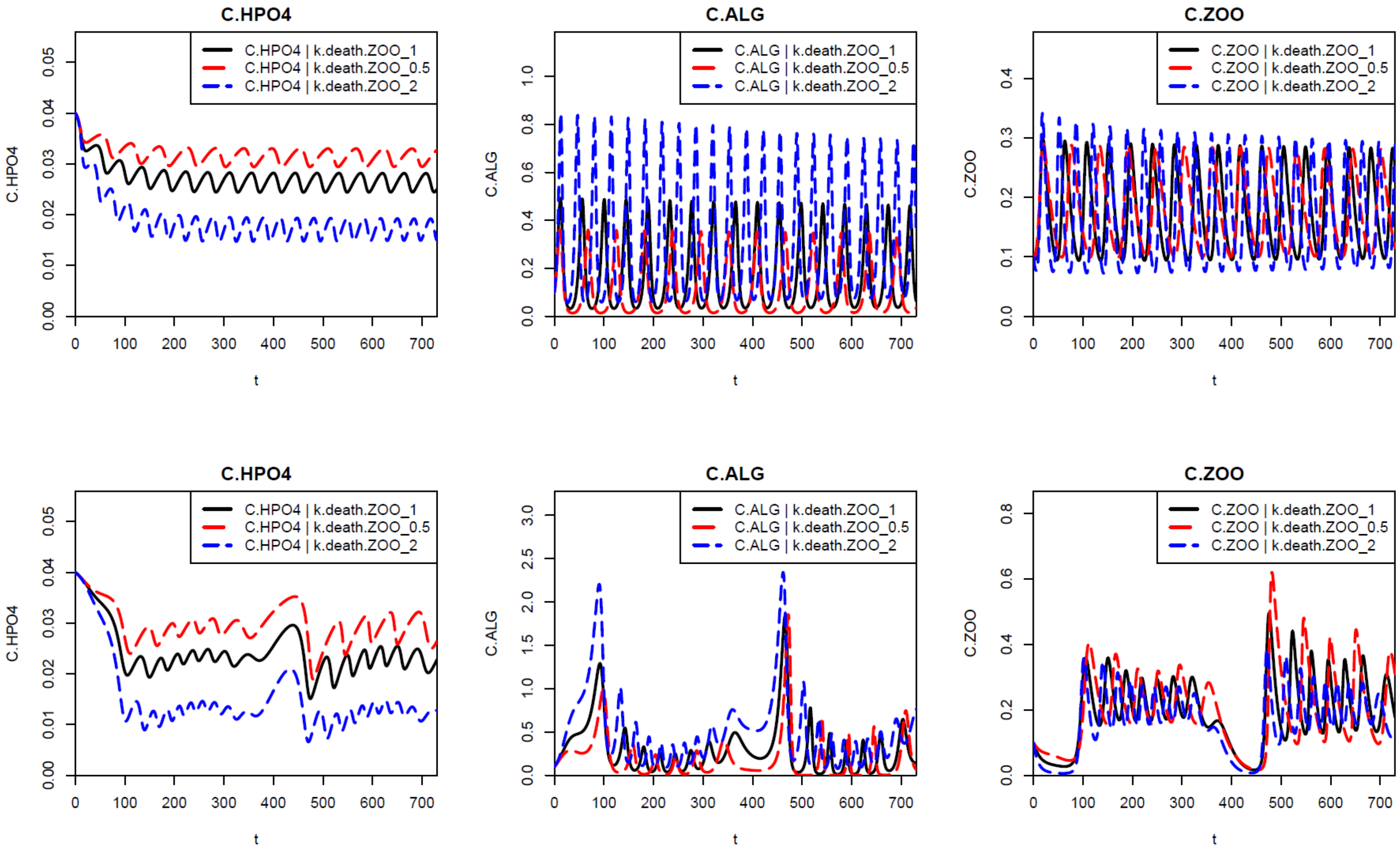
Review Exercise 2: Sensitivity Analysis



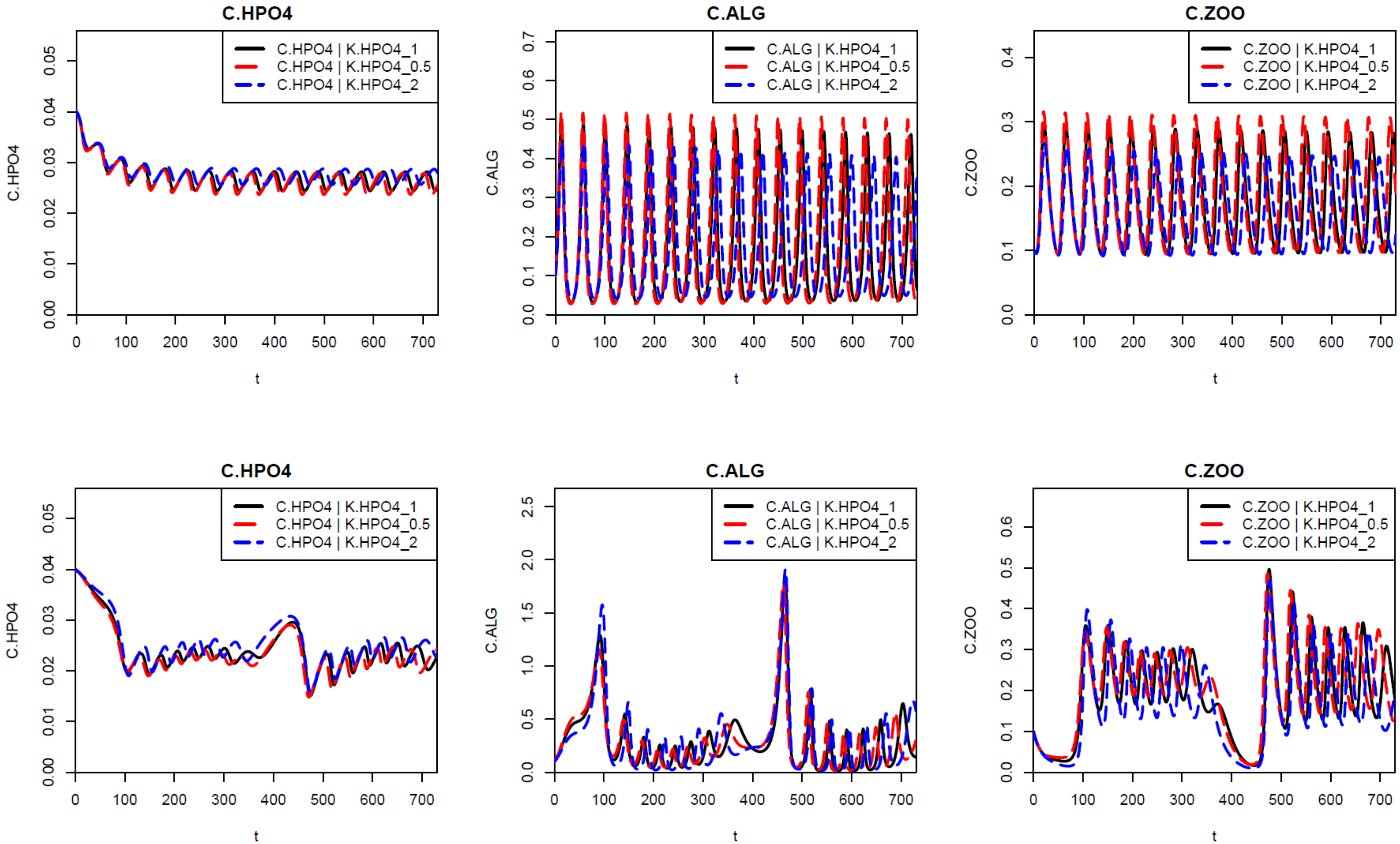
Review Exercise 2: Sensitivity Analysis



Review Exercise 2: Sensitivity Analysis



Review Exercise 2: Sensitivity Analysis



Review Exercise 2: Sensitivity Analysis

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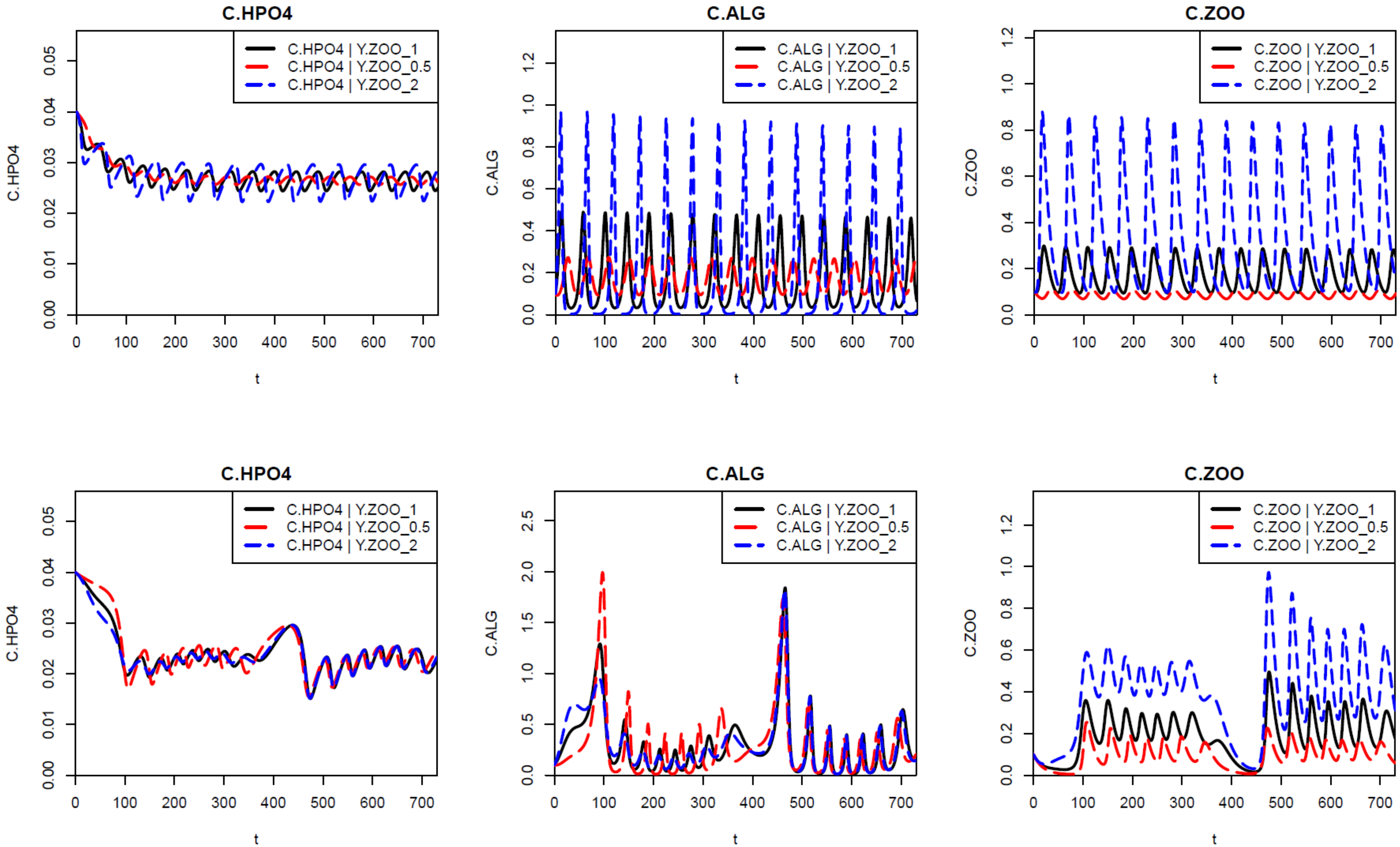
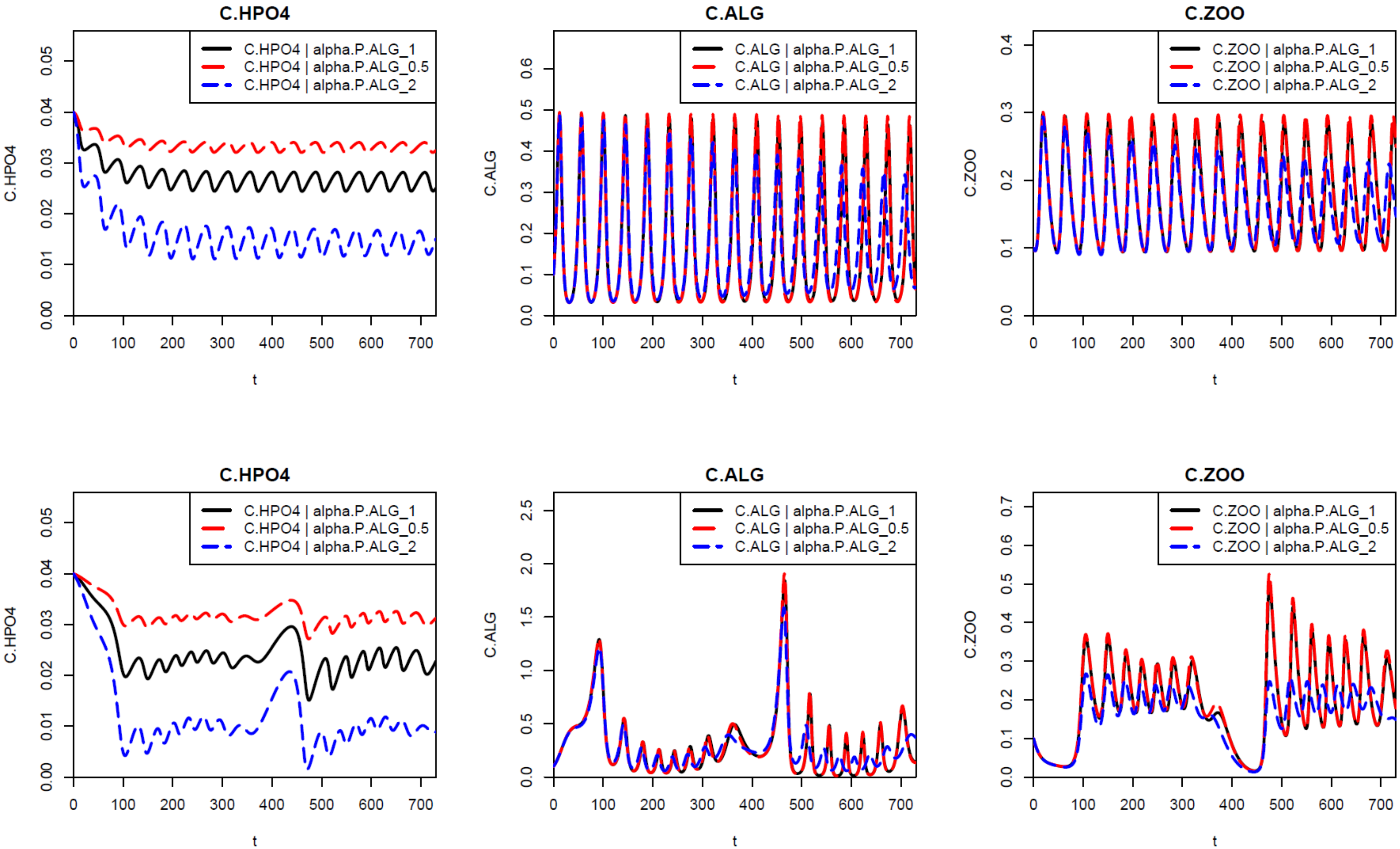


Review Exercise 2: Sensitivity Analysis



Review Exercise 2: Lessons learned?

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Stoichiometry

Process i	Substances j					Rate
	s_1	s_2	s_3	$\cdots$	$\mathsf{s}_{n_\mathrm{s}}$	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$\mathsf{p}_{n_\mathrm{p}}$	$\nu_{n_\mathrm{p}1}$	$\nu_{n_\mathrm{p}2}$	$\nu_{n_\mathrm{p}3}$	$\cdots$	$\nu_{n_\mathrm{p}n_\mathrm{s}}$	ρ_{n_p}

$$r_j = \sum_{i=1}^{n_\mathrm{p}} \nu_{ij}\ \rho_i$$

How to derive the stoichiometric coefficients ν_{ij}?

Stoichiometry: Ingredients for 1 cake?

Best recipe: https://tinyurl.com/Schoggikuchen

Process table for chocolate cake

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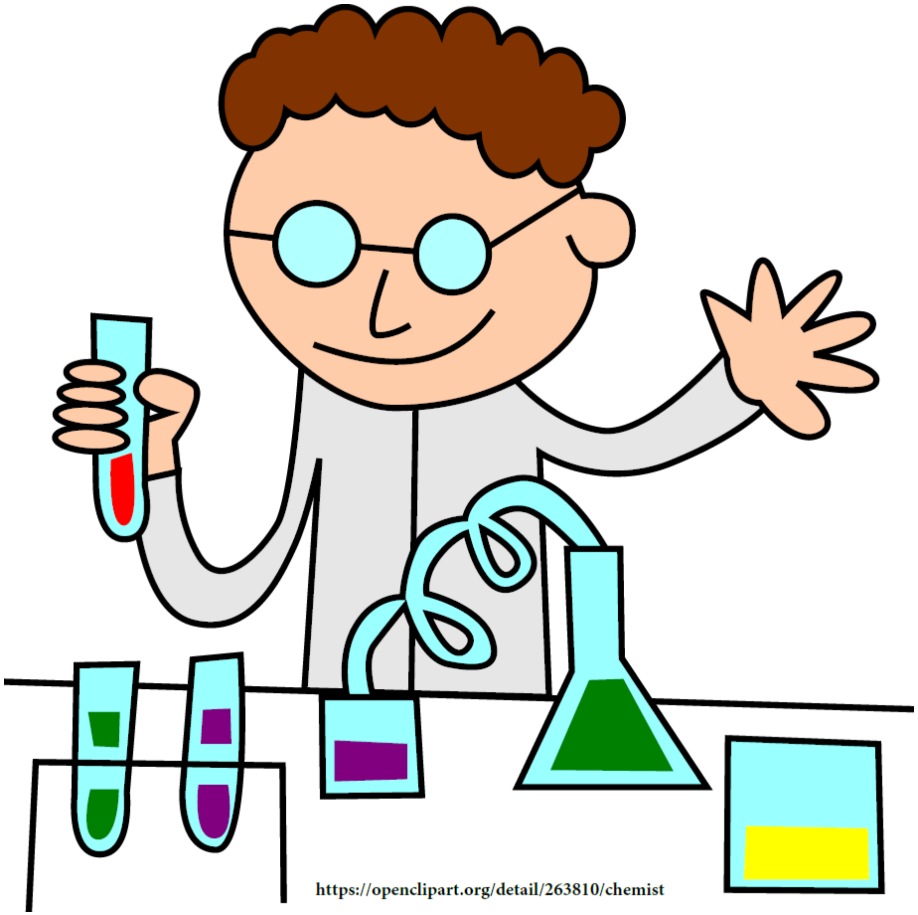
process	Chocolate [g]	Egg [no.]	Butter [g]	Sugar [g]	Cake [no.]	rate $[min^{-1}]$
baking a cake	-300	-5	-100	-100	+1	1/25 (at 180 °C)

Stoichiometry



https://openclipart.org/detail/263810/chemist

Stoichiometry

chapter 4.3.1

3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- Parameterized elemental mass fractions
- General solution

Chemical Substance Notation

Process	NH_4^+	NO_3^-	HPO_4^{2-}	O_2	ALG	ZOO	POM
	Substances / Organisms						
	mol	mol	mol	mol	gDM	gDM	gDM
Growth of ALG,NH4	?		?	?	1		
Growth of ALG,NO3		?	?	?	1		
Respiration of ALG	?		?	?	-1		
Death of ALG					-1		1
Growth of ZOO	?		?	?	?	1	?
Respiration of ZOO	?		?	?		-1	
Death of ZOO						-1	1

here just units of measurement of the different substances

Additional substances for calculation of the stoichiometric coefficients: HCO_3^-, H^+, H_2O

Chemical Substance Notation

1. Example: Growth of algae

Typical composition of marine algae (Redfield, 1958)

$$(CH_2O)_{106}(NH_3)_{16}(H_3PO_4)_1 = C_{106}H_{263}O_{110}N_{16}P$$

Total "molar" mass:

$$\begin{aligned} M &= 106 \cdot 12 \,\frac{\text{gC}}{\text{"mol"}} + 263 \,\frac{\text{gH}}{\text{"mol"}} + 110 \cdot 16 \,\frac{\text{gO}}{\text{"mol"}} \\ &\quad +16 \cdot 14 \,\frac{\text{gN}}{\text{"mol"}} + 31 \,\frac{\text{gP}}{\text{"mol"}} \\ &= 3550 \,\frac{\text{gDM}}{\text{"mol"}} \end{aligned}$$

Chemical Substance Notation

1. Example: Growth of algae with nitrate:

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

6 unknowns (a, b, c, d, e, f)

equations for the conservation of "mass": ?

Chemical Substance Notation

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1. Example: Growth of algae with nitrate:

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

6 unknowns (*a, b, c, d, e, f*)

equations for the conservation of "mass": for C, H, O, N, P and charge

C: $a \cdot 1 = 1 \cdot 106 \rightarrow a = 106$

Chemical Substance Notation

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1. Example: Growth of algae with nitrate:

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

6 unknowns (a, b, c, d, e, f)

equations for the conservation of "mass": for C, H, O, N, P and charge

C: $a \cdot 1 = 1 \cdot 106 \rightarrow a = 106$

N: $b \cdot 1 = 1 \cdot 16 \rightarrow b = 16$

Chemical Substance Notation

1. Example: Growth of algae with nitrate:

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

6 unknowns (a, b, c, d, e, f)

equations for the conservation of "mass": for C, H, O, N, P and charge

C: $a \cdot 1 = 1 \cdot 106 \rightarrow a = 106$

N: $b \cdot 1 = 1 \cdot 16 \rightarrow b = 16$

P: $c \cdot 1 = 1 \cdot 1 \rightarrow c = 1$

Chemical Substance Notation

1. Example: Growth of algae with nitrate:

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O$$
$$\rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

6 unknowns (*a, b, c, d, e, f*)

equations for the conservation of "mass": for C, H, O, N, P and charge

a = 106, *b* = 16, *c* = 1

H: $106 \cdot 1 + 1 \cdot 1 + d \cdot 1 + e \cdot 2 = 1 \cdot 263$,

O: $106 \cdot 3 + 16 \cdot 3 + 1 \cdot 4 + e \cdot 1 = 1 \cdot 110 + f \cdot 2$,

e⁻: $106 \cdot (-1) + 16 \cdot (-1) + 1 \cdot (-2) + d \cdot (+1) = 0$.

d =124 *e* =16 *f* =138

Chemical Substance Notation

1. Example: Growth of algae with nitrate:

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

a = 106, b = 16, c = 1, d = 124, e = 16, f = 138

$$106\,HCO_3^- + 16\,NO_3^- + HPO_4^{2-} + 124\,H^+ + 16\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + 138\,O_2$$

$$M_{ALG} = 3550\ \frac{\text{gDM}}{\text{“mol”}}$$

Chemical Substance Notation

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Stoichiometric coefficients for growth of algae:

$$\nu_{\text{gro,ALG,NO3 HCO}_3^-} = -\frac{106}{3550}\frac{\text{molHCO}_3^-}{\text{gDM}}$$

$$\nu_{\text{gro,ALG,NO3 NO}_3^-} = -\frac{16}{3550}\frac{\text{molNO}_3^-}{\text{gDM}}$$

$$\nu_{\text{gro,ALG,NO3 HPO}_4^{2-}} = -\frac{1}{3550}\frac{\text{molHPO}_4^{2-}}{\text{gDM}}$$

$$\nu_{\text{gro,ALG,NO3 H+}} = -\frac{124}{3550}\frac{\text{molH}^+}{\text{gDM}}$$

$$\nu_{\text{gro,ALG,NO3 H}_2\text{O}} = -\frac{16}{3550}\frac{\text{molH}_2\text{O}}{\text{gDM}}$$

$$\nu_{\text{gro,ALG,NO3 ALG}} = 1\frac{\text{gDM}}{\text{gDM}}$$

$$\nu_{\text{gro,ALG,NO3 O}_2} = \frac{138}{3550}\frac{\text{molO}_2}{\text{gDM}}$$

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Chemical Substance Notation

Do exercise L2 Task 1

$$a\,HCO_3^- + b\,NH_4^+ + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

Chemical Substance Notation

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Similarly for algal growth with ammonium:

$$106\,HCO_3^- + 16\,NH_4^+ + HPO_4^{2-} + 92\,H^+ \rightarrow C_{106}H_{263}O_{110}N_{16}P + 106\,O_2$$

Respiration:

$$C_{106}H_{263}O_{110}N_{16}P + 106\,O_2 \rightarrow 106\,HCO_3^- + 16\,NH_4^+ + HPO_4^{2-} + 92\,H^+$$

Death:

$$C_{106}H_{263}O_{110}N_{16}P \rightarrow C_{106}H_{263}O_{110}N_{16}P$$

Chemical Substance Notation

Process	Substances / Organisms						
	NH_4^+ mol	NO_3^- mol	HPO_4^{2-} mol	O_2 mol	ALG gDM	ZOO gDM	POM gDM
Growth of ALG,NH4	?		?	?	1		
Growth of ALG,NO3		?	?	?	1		
Respiration of ALG	?		?	?	-1		
Death of ALG					-1		1
Growth of ZOO	?		?	?	?	1	?
Respiration of ZOO	?		?	?		-1	
Death of ZOO						-1	1

→ how many unknowns?

Additional substances for calculation of the stoichiometric coefficients:
HCO_3^-, H^+, H_2O

Chemical Substance Notation

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Zooplankton Growth:

8 unknown stoichiometric coefficients

6 mass balance equations

2 additional constraints required:

Fraction of zooplankton biomass produced per algal biomass consumed (yield): Y_{ZOO}

Fraction of dead particles produced (excretion + sloppy feeding) per algal biomass consumed: f_{e}

The fraction of algal biomass respired is then: $f_{\mathrm{r}} = 1 - Y_{\mathrm{ZOO}} - f_{\mathrm{e}}$

Chemical Substance Notation

Process	NH_4^+ mol	NO_3^- mol	HPO_4^{2-} mol	O_2 mol	ALG gDM	ZOO gDM	POM gDM
	Substances / Organisms						
Gro. ALG,NH4	$-\frac{16}{3550}$		$-\frac{1}{3550}$	$\frac{106}{3550}$	1		
Gro. ALG,NO3		$-\frac{16}{3550}$	$-\frac{1}{3550}$	$\frac{138}{3550}$	1		
Resp. ALG	$\frac{16}{3550}$		$\frac{1}{3550}$	$-\frac{106}{3550}$	-1		
Death ALG					-1		1
Growth ZOO	$\frac{f_r}{Y_{ZOO}} \frac{16}{3550}$		$\frac{f_r}{Y_{ZOO}} \frac{1}{3550}$	$-\frac{f_r}{Y_{ZOO}} \frac{106}{3550}$	$-\frac{1}{Y_{ZOO}}$	1	$\frac{f_e}{Y_{ZOO}}$
Resp. ZOO	$\frac{16}{3550}$		$\frac{1}{3550}$	$-\frac{106}{3550}$		-1	
Death ZOO						-1	1

Chemical Substance Notation:

Quite some handwork!

If composition changes: redo the calculation!

→ instead of fixed composition use parameters for elemental mass fractions

Stoichiometry

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chapter 4.3.2

3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- Parameterized elemental mass fractions
- General solution

Extended Process Table Notation

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Processes i	Substances j					Rates
	s_1	s_2	s_3	$\cdots$	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
p_{n_p}	ν_{n_p1}	ν_{n_p2}	ν_{n_p3}	$\cdots$	$\nu_{n_pn_s}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	$\cdots$	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	$\cdots$	α_{2n_s}	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	
e_{n_e}	α_{n_e1}	α_{n_e2}	α_{n_e3}	$\cdots$	$\alpha_{n_en_s}$	

ν_{ij}: stoich. coeff. = relative transf. rate of substance j in proc. i

α_{kj}: mass fraction of element k on substance j

$\nu_{ij}\alpha_{kj}$: relative transf. rate of element k contained in subst. j

Extended Process Table Notation

Processes i	Substances j					Rates
	s_1	s_2	s_3	$\cdots$	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
p_{n_p}	ν_{n_p1}	ν_{n_p2}	ν_{n_p3}	$\cdots$	$\nu_{n_pn_s}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	$\cdots$	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	$\cdots$	α_{2n_s}	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	
e_{n_e}	α_{n_e1}	α_{n_e2}	α_{n_e3}	$\cdots$	$\alpha_{n_en_s}$	

Mass conservation for element k in process i: $\boxed{\sum_j \nu_{ij}\alpha_{kj} = 0}$

Parameterized Mass Fractions

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Process	Substances / Organisms						
	NH_4^+ mol	NO_3^- mol	HPO_4^{2-} mol	O_2 mol	ALG gDM	ZOO gDM	POM gDM
Growth of ALG,NH4	?		?	?	1		
Growth of ALG,NO3		?	?	?	1		
Respiration of ALG	?		?	?	-1		
Death of ALG					-1		1
Growth of ZOO	?		?	?	?	1	?
Respiration of ZOO	?		?	?		-1	
Death of ZOO						-1	1

Additional substances for calculation of the stoichiometric coefficients:
HCO_3^-, H^+, H_2O

Mass balance equations for C,H,O,N,P and charge

Parameterized Mass Fractions

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Instead of assuming a fixed chemical composition (e.g. Redfield:)

$$C_{106}H_{263}O_{110}N_{16}P$$

use parameterized mass fractions:

$$C_{\alpha_{C,j}/12}H_{\alpha_{H,j}}O_{\alpha_{O,j}/16}N_{\alpha_{N,j}/14}P_{\alpha_{P,j}/31}$$

with:

$$\alpha_{C,j} + \alpha_{H,j} + \alpha_{O,j} + \alpha_{N,j} + \alpha_{P,j} = 1$$

Parameterized Mass Fractions

Redfield composition:

$$\alpha_{\mathrm{C,ALG}}^{\mathrm{Redfield}} = \frac{106 \cdot 12}{3550} \frac{\mathrm{gC}}{\mathrm{gDM}} \approx 0.36 \frac{\mathrm{gC}}{\mathrm{gDM}}$$

$$\alpha_{\mathrm{H,ALG}}^{\mathrm{Redfield}} = \frac{263}{3550} \frac{\mathrm{gH}}{\mathrm{gDM}} \approx 0.07 \frac{\mathrm{gH}}{\mathrm{gDM}}$$

$$\alpha_{\mathrm{O,ALG}}^{\mathrm{Redfield}} = \frac{110 \cdot 16}{3550} \frac{\mathrm{gO}}{\mathrm{gDM}} \approx 0.50 \frac{\mathrm{gO}}{\mathrm{gDM}}$$

$$\alpha_{\mathrm{N,ALG}}^{\mathrm{Redfield}} = \frac{16 \cdot 14}{3550} \frac{\mathrm{gN}}{\mathrm{gDM}} \approx 0.06 \frac{\mathrm{gN}}{\mathrm{gDM}}$$

$$\alpha_{\mathrm{P,ALG}}^{\mathrm{Redfield}} = \frac{1 \cdot 31}{3550} \frac{\mathrm{gP}}{\mathrm{gDM}} \approx 0.01 \frac{\mathrm{gP}}{\mathrm{gDM}}$$

Parameterized Mass Fractions

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \\ \rightarrow C_{106}H_{263}O_{110}N_{16}P + f\,O_2$$

Setting up equation for algal growth with unknown coefficients:

$$a\,HCO_3^- + b\,NO_3^- + c\,HPO_4^{2-} + d\,H^+ + e\,H_2O \\ \rightarrow C_{\alpha_{C,ALG}/12}H_{\alpha_{H,ALG}}O_{\alpha_{O,ALG}/16}N_{\alpha_{N,ALG}/14}P_{\alpha_{P,ALG}/31} + f\,O_2$$

Conservation of C: $a = \frac{\alpha_{C,ALG}}{12}$

Conservation of N: $b = \frac{\alpha_{N,ALG}}{14}$

Conservation of P: $c = \frac{\alpha_{P,ALG}}{31}$

Parameterized Mass Fractions

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$$\frac{\alpha_{C,ALG}}{12} HCO_3^- + \frac{\alpha_{N,ALG}}{14} NO_3^- + \frac{\alpha_{P,ALG}}{31} HPO_4^{2-} + d\,H^+ + e\,H_2O$$
$$\rightarrow C_{\alpha_{C,ALG}/12} H_{\alpha_{H,ALG}} O_{\alpha_{O,ALG}/16} N_{\alpha_{N,ALG}/14} P_{\alpha_{P,ALG}/31} + f\,O_2$$

Conservation of H, O and charge:

H: $\frac{\alpha_{C,ALG}}{12} \cdot 1 + \frac{\alpha_{P,ALG}}{31} \cdot 1 + d \cdot 1 + e \cdot 2 = 1 \cdot \alpha_{H,ALG}$

O: $\frac{\alpha_{C,ALG}}{12} \cdot 3 + \frac{\alpha_{N,ALG}}{14} \cdot 3 + \frac{\alpha_{P,ALG}}{31} \cdot 4 + e \cdot 1 = 1 \cdot \frac{\alpha_{O,ALG}}{16} + f \cdot 2$

charge: $\frac{\alpha_{C,ALG}}{12} \cdot (-1) + \frac{\alpha_{N,ALG}}{14} \cdot (-1) + \frac{\alpha_{P,ALG}}{31} \cdot (-2) + d \cdot (+1) = 0$

Parameterized Mass Fractions

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$$d = \frac{\alpha_{\mathrm{C,ALG}}}{12} + \frac{\alpha_{\mathrm{N,ALG}}}{14} + \frac{2\ \alpha_{\mathrm{P,ALG}}}{31}$$

$$e = \frac{\alpha_{\mathrm{H,ALG}}}{2} - \frac{\alpha_{\mathrm{C,ALG}}}{12} - \frac{\alpha_{\mathrm{N,ALG}}}{28} - \frac{3\ \alpha_{\mathrm{P,ALG}}}{62}$$

$$f = \frac{\alpha_{\mathrm{C,ALG}}}{12} + \frac{\alpha_{\mathrm{H,ALG}}}{4} - \frac{\alpha_{\mathrm{O,ALG}}}{32} + \frac{5\ \alpha_{\mathrm{N,ALG}}}{56} + \frac{5\ \alpha_{\mathrm{P,ALG}}}{124}$$

Parameterized Mass Fractions

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Growth of algae:

$$\frac{\alpha_{\mathrm{C,ALG}}}{12}\,\mathrm{HCO_3^-} + \frac{\alpha_{\mathrm{N,ALG}}}{14}\,\mathrm{NO_3^-} + \frac{\alpha_{\mathrm{P,ALG}}}{31}\,\mathrm{HPO_4^{2-}}$$

$$+ \left(\frac{\alpha_{\mathrm{C,ALG}}}{12} + \frac{\alpha_{\mathrm{N,ALG}}}{14} + \frac{2\,\alpha_{\mathrm{P,ALG}}}{31}\right)\mathrm{H^+}$$

$$+ \left(\frac{\alpha_{\mathrm{H,ALG}}}{2} - \frac{\alpha_{\mathrm{C,ALG}}}{12} - \frac{\alpha_{\mathrm{N,ALG}}}{28} - \frac{3\,\alpha_{\mathrm{P,ALG}}}{62}\right)\mathrm{H_2O}$$

$$\rightarrow \mathrm{C}_{\alpha_{\mathrm{C,ALG}}/12}\mathrm{H}_{\alpha_{\mathrm{H,ALG}}}\mathrm{O}_{\alpha_{\mathrm{O,ALG}}/16}\mathrm{N}_{\alpha_{\mathrm{N,ALG}}/14}\mathrm{P}_{\alpha_{\mathrm{P,ALG}}/31}$$

$$+ \left(\frac{\alpha_{\mathrm{C,ALG}}}{12} + \frac{\alpha_{\mathrm{H,ALG}}}{4} - \frac{\alpha_{\mathrm{O,ALG}}}{32} + \frac{5\,\alpha_{\mathrm{N,ALG}}}{56} + \frac{5\,\alpha_{\mathrm{P,ALG}}}{124}\right)\mathrm{O_2}$$

Parameterized Mass Fractions

Do exercise L2 Task 2

Parameterized Mass Fractions:

Changes in composition are now easy to handle,
just change the numerical values of the parameters.

What about adding additional elements?

The equations must be revised.

This is a laborious process.

Is there a general solution to this process?

→ Swiss Army Knife of Linear Algebra

Homework

1. Find out what the Swiss Army Knife of Linear Algebra is (hint: SVD)

2. Read chapter 4.3.3

3. Read chapter 14

4. Think about your open questions

5. Bonus: Try out the chocolate cake recipe

Structure of the Course

1. Introduction, principles of modelling environmental systems, mass balance in a mixed reactor, process table notation, simple lake plankton model
   Exercise: R, `ecosim`-package, simple lake plankton model
   Exercise: lake phytoplankton-zooplankton model
2. Process stoichiometry Exercises: analytical solution, calculation with `stoichcalc`
3. Biological processes in lakes
4. Physical processes in lakes, mass balance in multi-box and continuous systems Exercise: structured, biogeochemical-ecological lake model
   Assignments: build your own model by implementing model extensions
5. Physical processes in in rivers, bacterial growth, river model for benthic populations Exercise: river model for benthic populations, nutrients and oxygen
6. Stochasticity, uncertainty, Parameter estimation
   Exercise: uncertainty, stochasticity
7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback