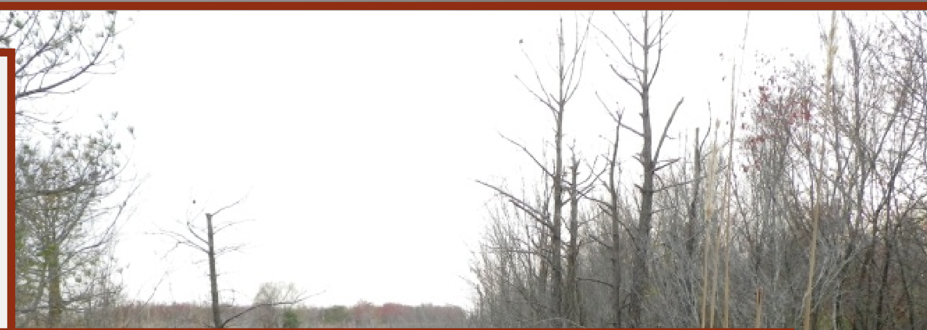
A generalized model of aquatic microbial metabolism based on thermodynamic, kinetic, and stoichiometric theory

Robert A. Payn[1,2]
Ashley M. Helton[3]
Geoffrey C. Poole[1,2,4]
Clemente Izurieta[2,4]
Emily S. Bernhardt[3]
Amy J. Burgin[5]

1. *Department of Land Resources and Environmental Sciences, Montana State University*
2. *Institute on Ecosystems, Montana University System*
3. *Biology Department, Duke University*
4. *Computer Science Department, Montana State University*
5. *School of Natural Resources, University of Nebraska - Lincoln*

A generalized model of aquatic microbial metabolism based on th

stoi



Rob
Ashl
Geoff
Clem
Emily
An

ersity
-

Timberlake Wetland Restoration Project

Privately owned carbon mitigation bank

Row-crop agricultural land starting in 1985, drained by active surface water pumping

Native vegetation restored and reflooded in 2007

Seasonal brackish surface water intrusion driven by wind tides

Timberlake Wetland Restoration Project

Overarching biogeochemical questions:

What is the state and trajectory of nutrient and trace gas emissions resulting from the restoration?

How might this state and trajectory be altered by brackish water influence (e.g. influence of sulfate)?

Timberlake Wetland Restoration Project

Question at hand:

How do we predict the trajectory when we cannot interpolate from former states of the system?

Approach:

Mechanistic modeling of microbial metabolism in soils

Timberlake Wetland Restoration Project

Challenge:

Existing models are too detailed for typical whole-ecosystem methods

Data on specific enzymes and microbial species are impractical for whole-system predictions

Futures 1994 26(6) 626–647

COMPLEXITY A
TH

To

Eric

Metabolic process	Reaction	$E_S = -\Delta G_r^0$ (kJ mol^{-1})
Aerobic organic carbon oxidation	$CH_2O + O_2 \leftrightarrow CO_2 + H_2O$	502

TABLE 1. CHARACTERISTICS OF ECOSYSTEM GROWTH AND DEVELOPMENT

As ecosystem organization increases, grows and develops we expect the following system changes (the appropriate measures are in italics):

1. More energy capture. *Inflow*
2. More effective use of energy. *Exergy destruction rate*
3. More energy flow activity within the system. *Total system throughput (TST)*
4. More cycling of energy and material:
   (a) Greater number of cycles; *number of cycles*
   (b) Longer cycles; *average cycle length*
   (c) The amount of material flowing in cycles (as v straight-through flow) increases; *Finn cycling index*
   (d) Turnover time of cycles, or cycling rate, decreases; *decrease in production/biomass (P/B) ratio*
   (e) Less leaking of material out of the ecosystem. *Exports*
5. Higher average trophic structure:
   (a) Longer trophic food chains; *number of trophic levels in the Lindemann spine*
   (b) Species will occupy higher *average trophic levels*
   (c) Greater *trophic efficiencies*
6. More articulated food web. *Ascendancy*
7. Higher *respiration*
8. Higher *transpiration* in terrestrial systems
9. Larger ecosystem *biomass*
10. More types of organisms. *Diversity*

Growth optimization

$$\sum_{i=1}^{n} m_{S,i} E_{S,i} = m_M \frac{B_t + B_{t+\Delta t}}{2} + \sum_{j=1}^{n_G} m_{G,j} G_j$$

Sum of energy from reactions

Energy needed to maintain biomass

Energy needed to produce biomass

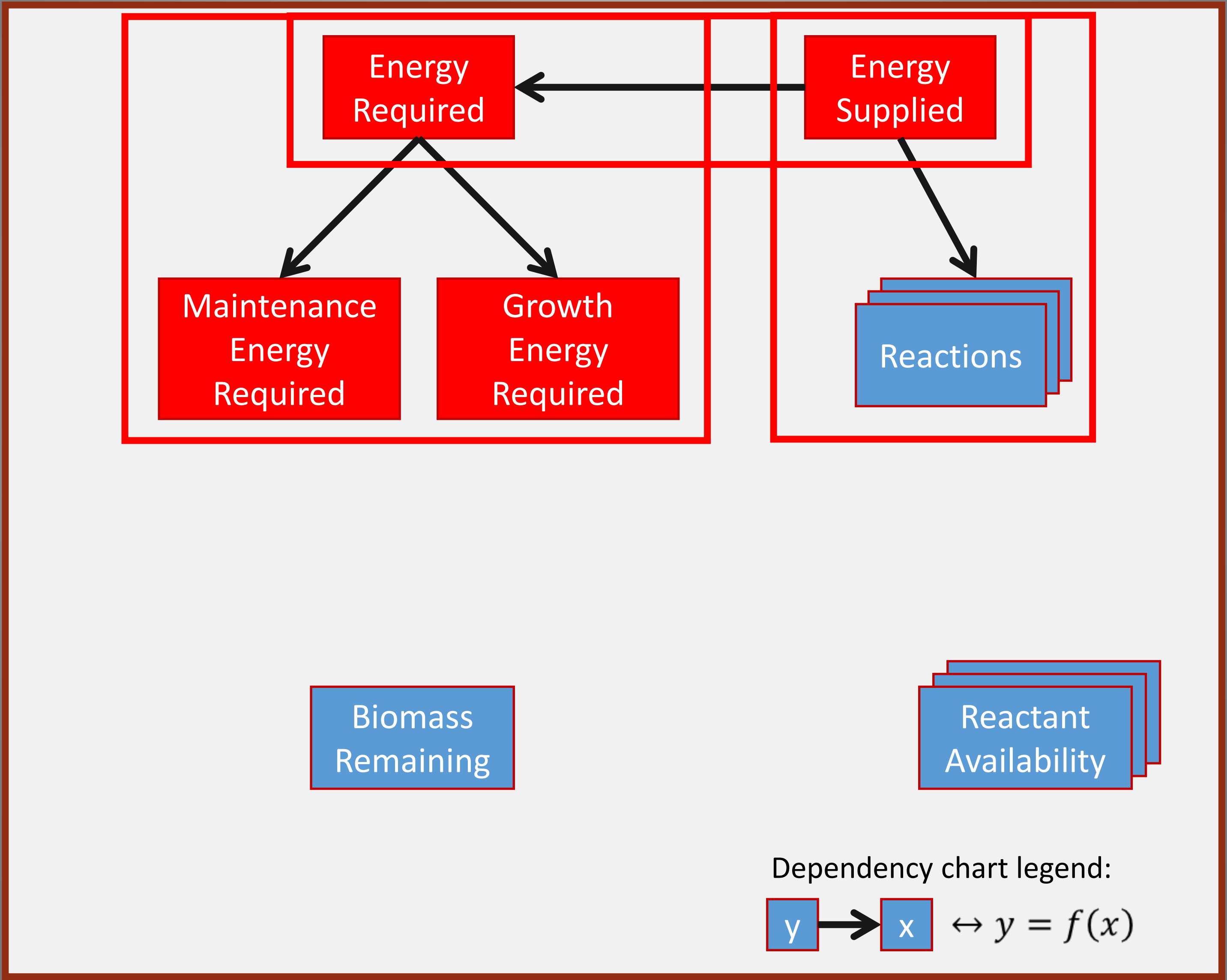
Biomass Remaining

Reactant Availability

Dependency chart legend:

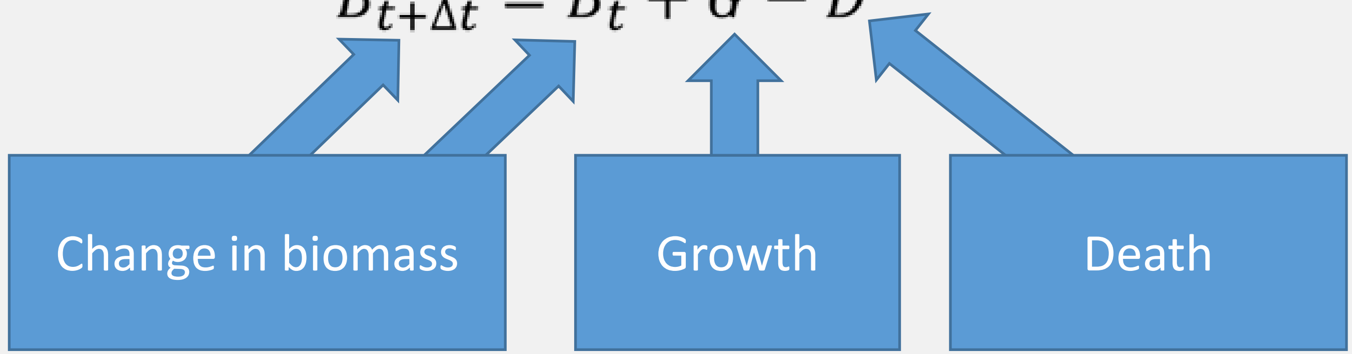
y → x $\leftrightarrow y = f(x)$

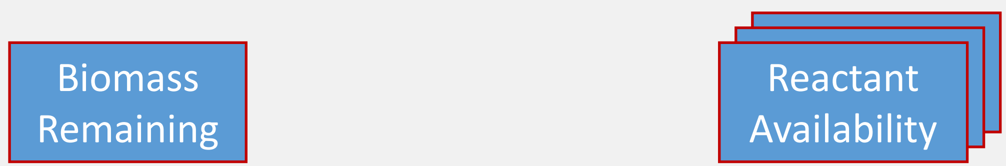
Growth optimization: energy balance



Growth optimization: mass balance biomass

$$B_{t+\Delta t} = B_t + G - D$$

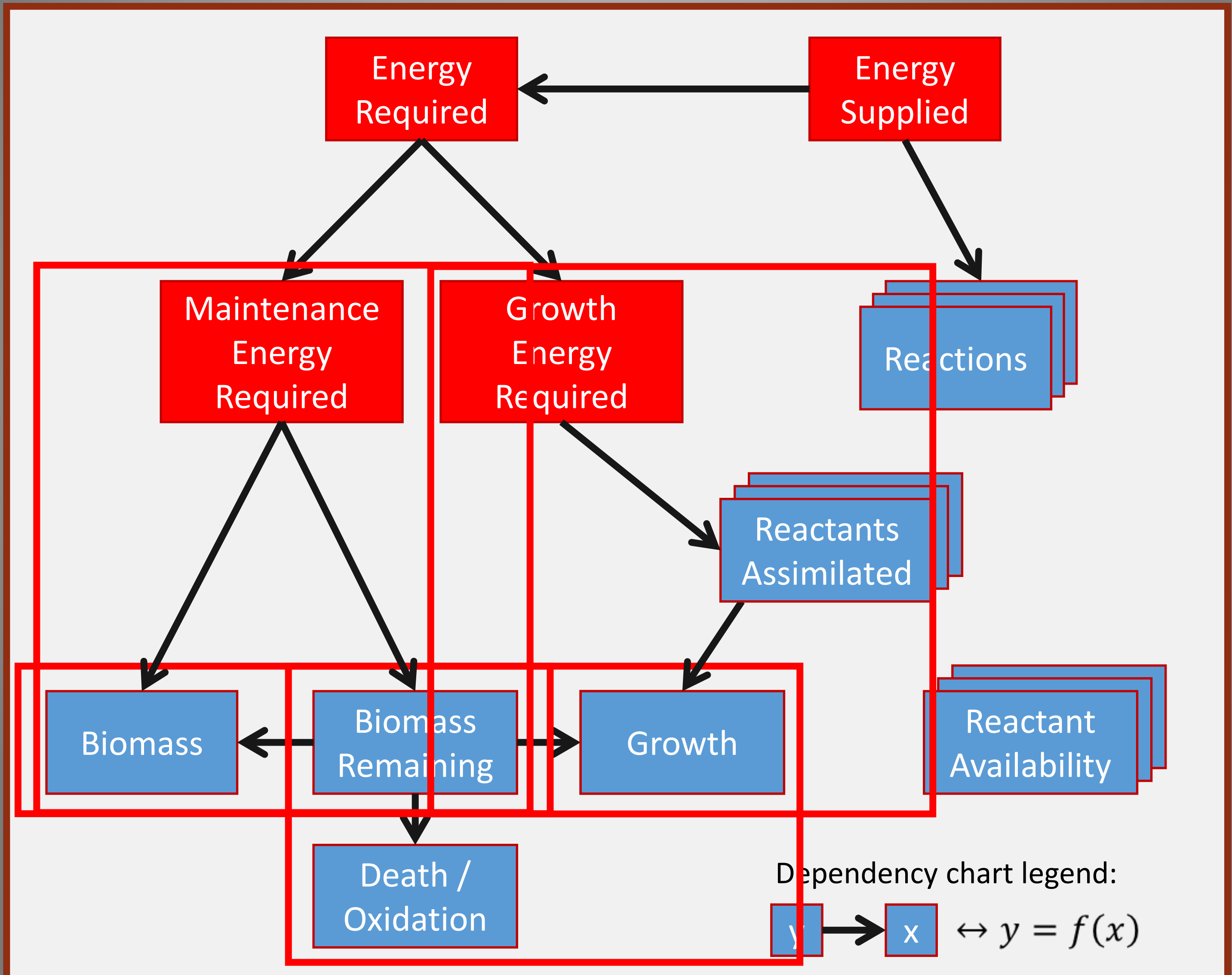




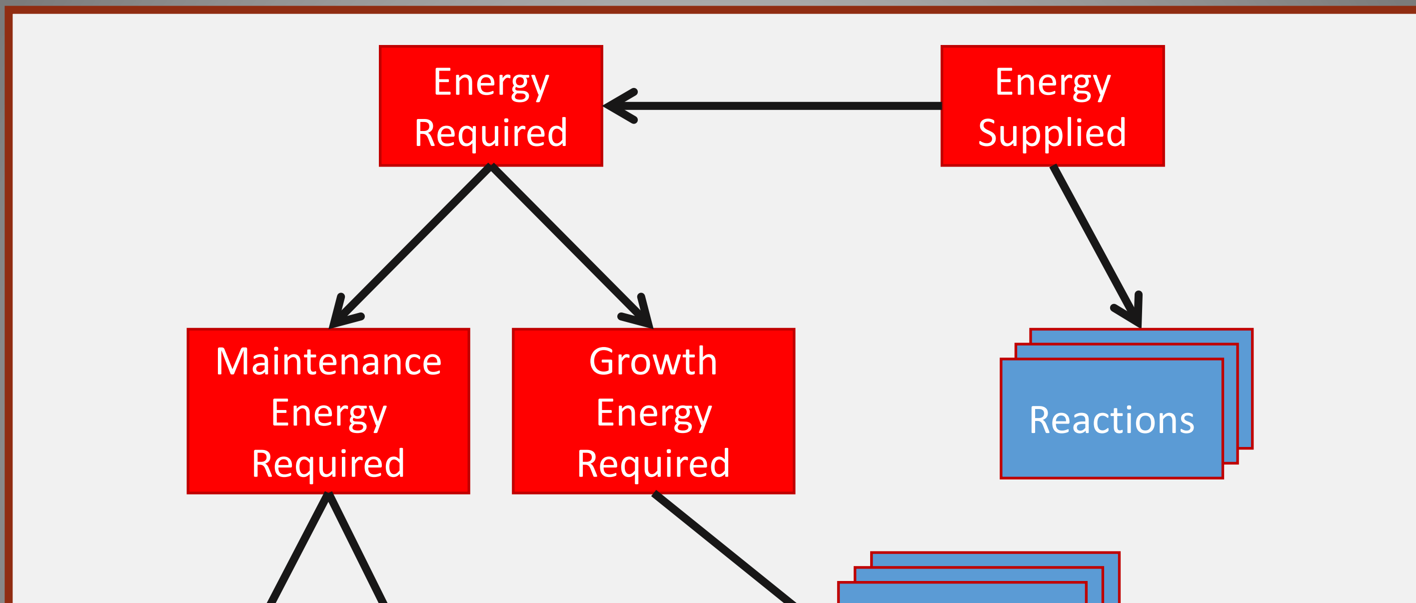
Dependency chart legend:

$y \rightarrow x \leftrightarrow y = f(x)$

Growth optimization: mass balance biomass



Growth optimization: mass balance compounds



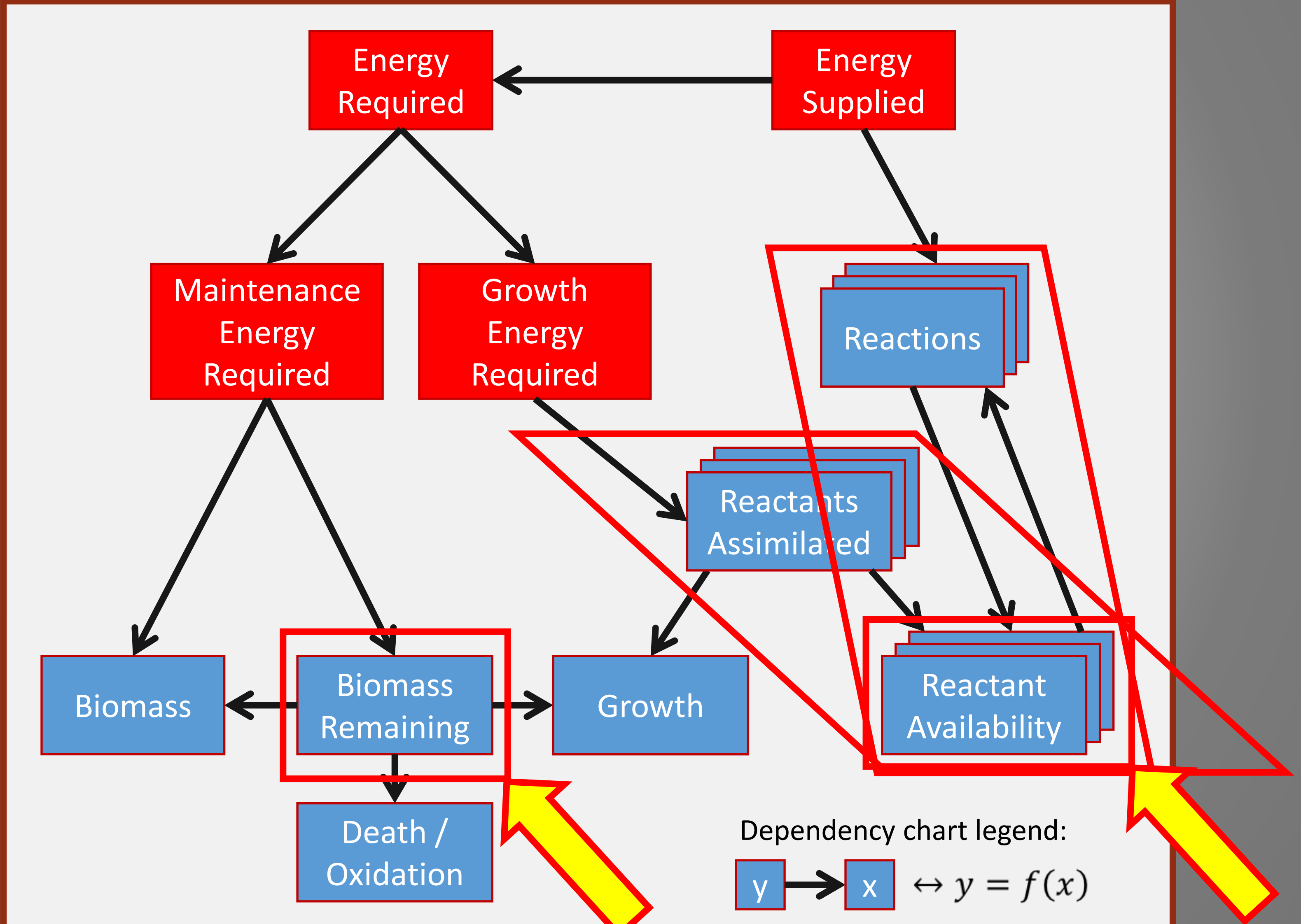
$$X_{t+\Delta t} = X_t + \sum_{i=1}^{n} f_{XP,i} m_{S,i} - \sum_{i=1}^{n} f_{XR,i} m_{S,i} - \sum_{j=1}^{n_G} f_{XG,i} G$$

Change in availability of the reactant

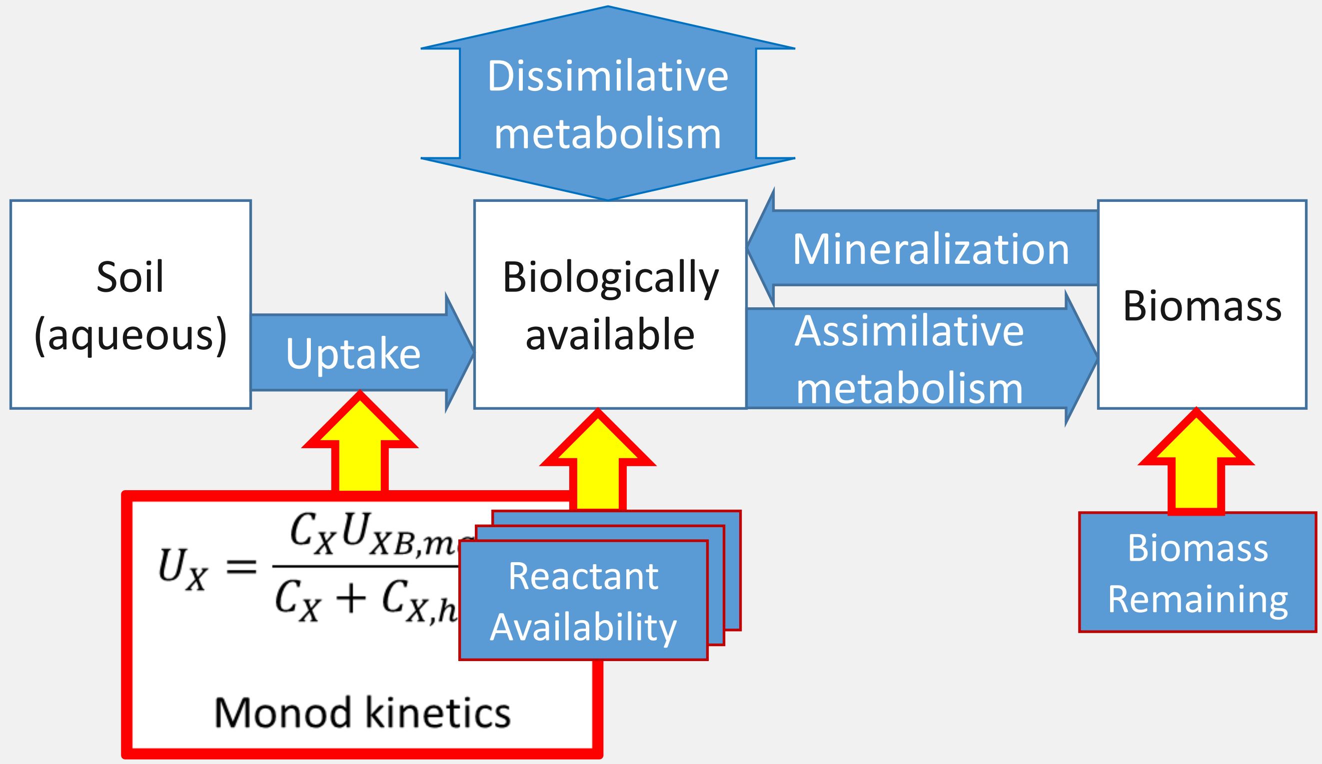
Amount of reactant produced or consumed in reactions

Assimilation of reactant

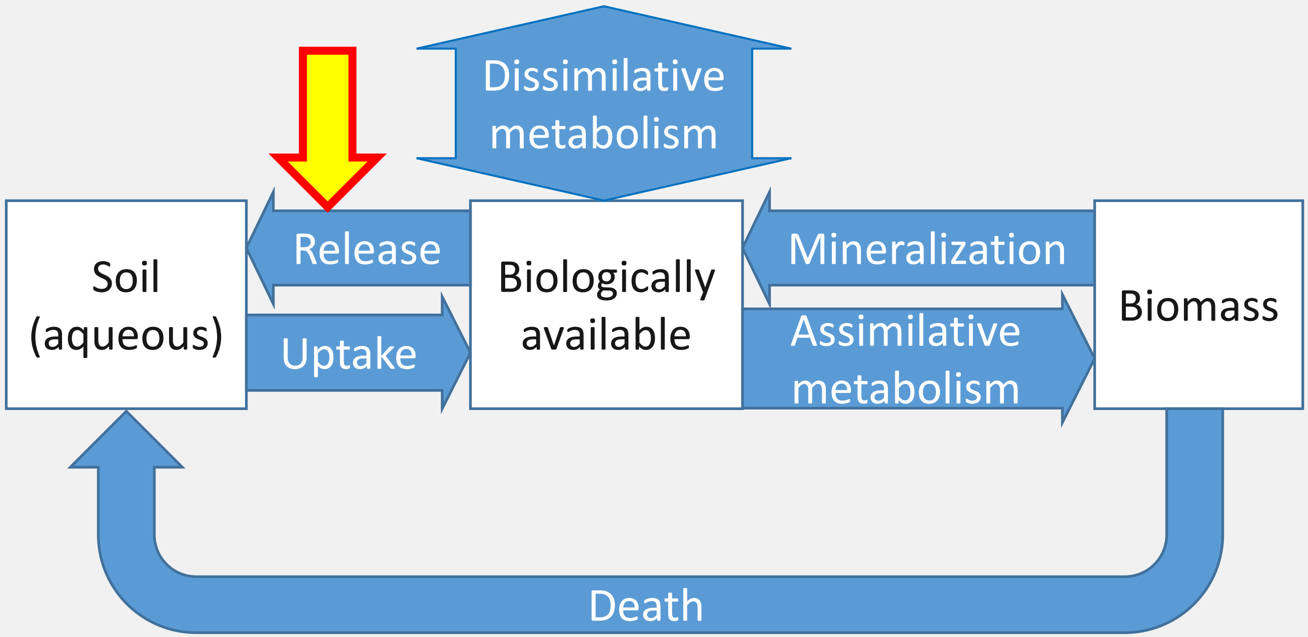
Growth optimization: mass balance compounds



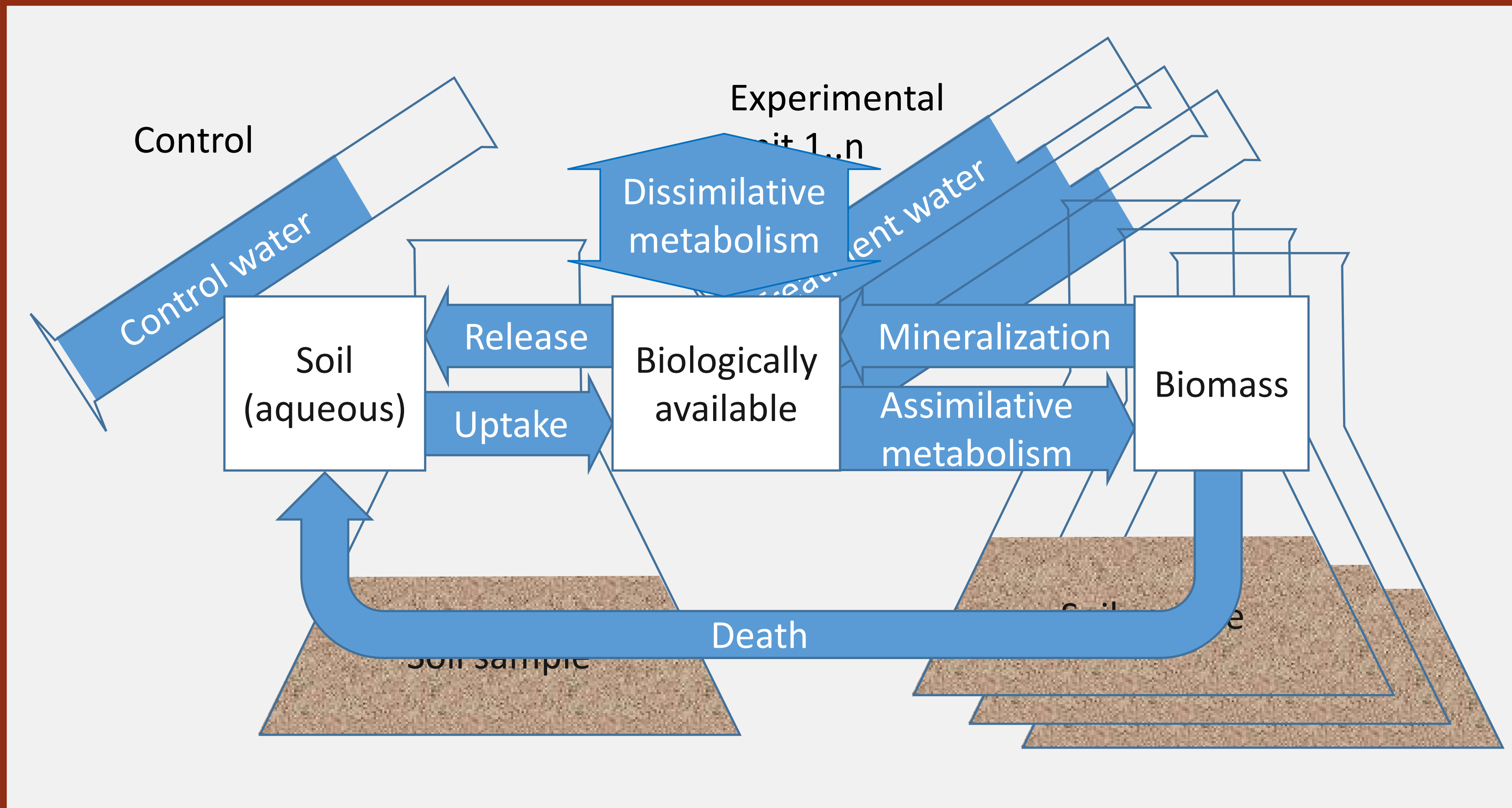
Simulation model



Simulation model



Batch reactor simulations



Batch reactor simulations: parameters

Variable	Value	Unit
Monod parameters		
$U_{XB,max}$	0.435	(mmol X) (mmol C biomass)$^{-1}$ hr^{-1}
$C_{X,half}$	2.83	mmol L^{-1}

Peil and Gaudy, Jr., 1971

Batch reactor simulations: parameters

Variable	Value	Unit
Monod parameters		
$U_{XB,max}$	0.435	(mmol X) (mmol C biomass)$^{-1}$ hr^{-1}
$C_{X,half}$	2.83	mmol L^{-1}
Energy demand		
E_{RM}	2.83	kJ (mol C biomass)$^{-1}$ hr^{-1}

Tijhuis et al., 1971

Batch reactor simulations: parameters

Variable	Value	Unit
Monod parameters		
$U_{XB,max}$	0.435	(mmol X) (mmol C biomass)$^{-1}$ hr^{-1}
$C_{X,half}$	2.83	mmol L^{-1}
Energy demand		
E_{RM}	2.83	kJ (mol C biomass)$^{-1}$ hr^{-1}
$E_{RG,auto}$	3500	kJ (mol C growth)$^{-1}$
$E_{RG,hetero}$	285	kJ (mol C growth)$^{-1}$
$E_{RG,methano}$	661	kJ (mol C growth)$^{-1}$

Tijhuis et al., 1971

Batch reactor simulations: parameters

Variable	Value	Unit
Monod parameters		
$U_{XB,max}$	0.435	(mmol X) (mmol C biomass)$^{-1}$ hr^{-1}
$C_{X,half}$	2.83	mmol L^{-1}
Energy demand		
E_{RM}	2.83	kJ (mol C biomass)$^{-1}$ hr^{-1}
$E_{RG,auto}$	3500	kJ (mol C growth)$^{-1}$
$E_{RG,hetero}$	285	kJ (mol C growth)$^{-1}$
$E_{RG,methano}$	661	kJ (mol C growth)$^{-1}$
$E_{RG,DON}$	0	kJ (mol N assimilated)$^{-1}$
$E_{RG,ammon}$	31	kJ (mol N assimilated)$^{-1}$
$E_{RG,nitrite}$	123.6	kJ (mol N assimilated)$^{-1}$
$E_{RG,nitrate}$	154.5	kJ (mol N assimilated)$^{-1}$

Model demonstration: thermodynamics

Favor heterotrophic reactions

Initial biomass = 0.56 mmol C

SIR analysis of Timberlake sample site 601

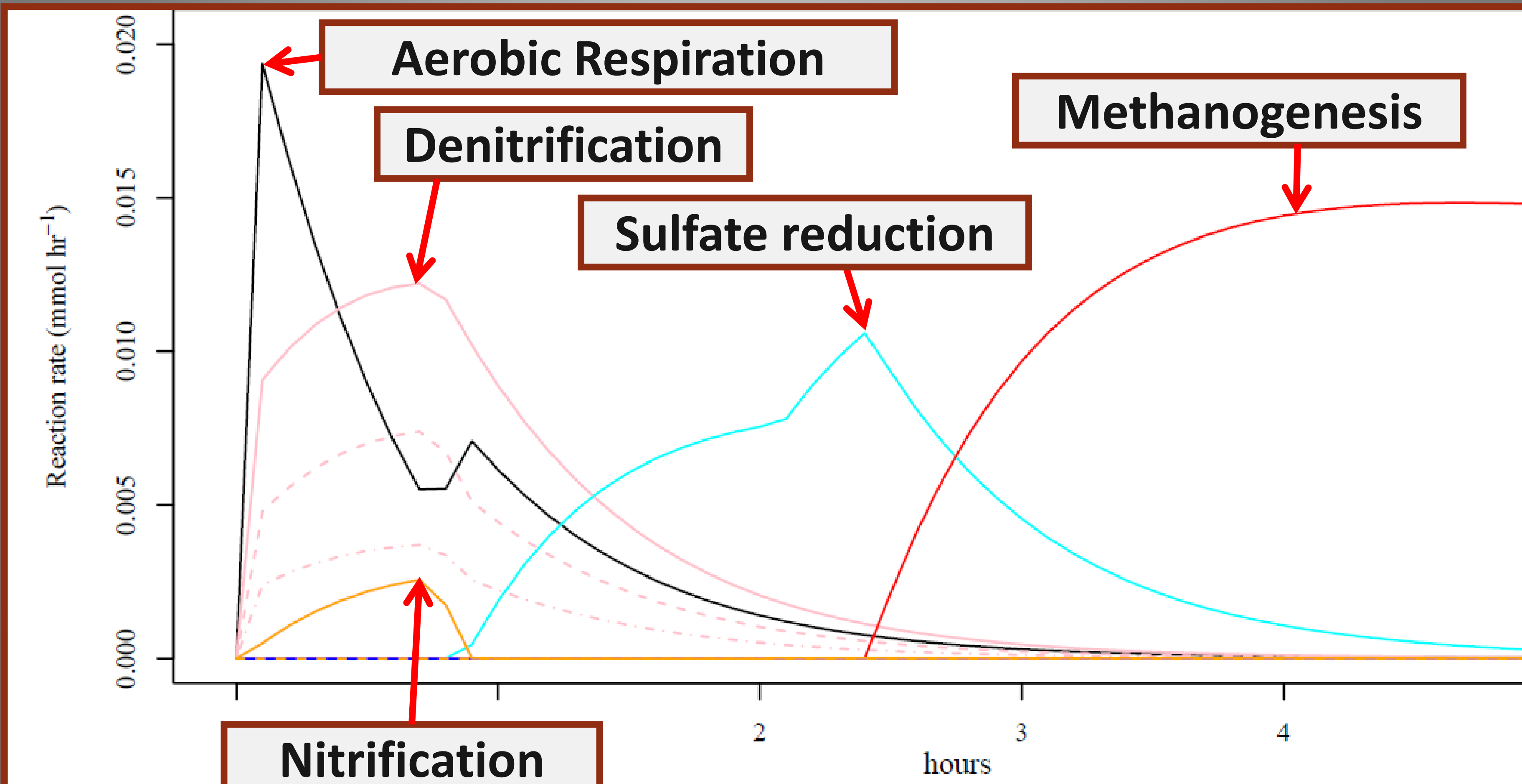
Initial DOC = 1.3 mmol C L^{-1}

Soil water extractions from Timberlake site 601

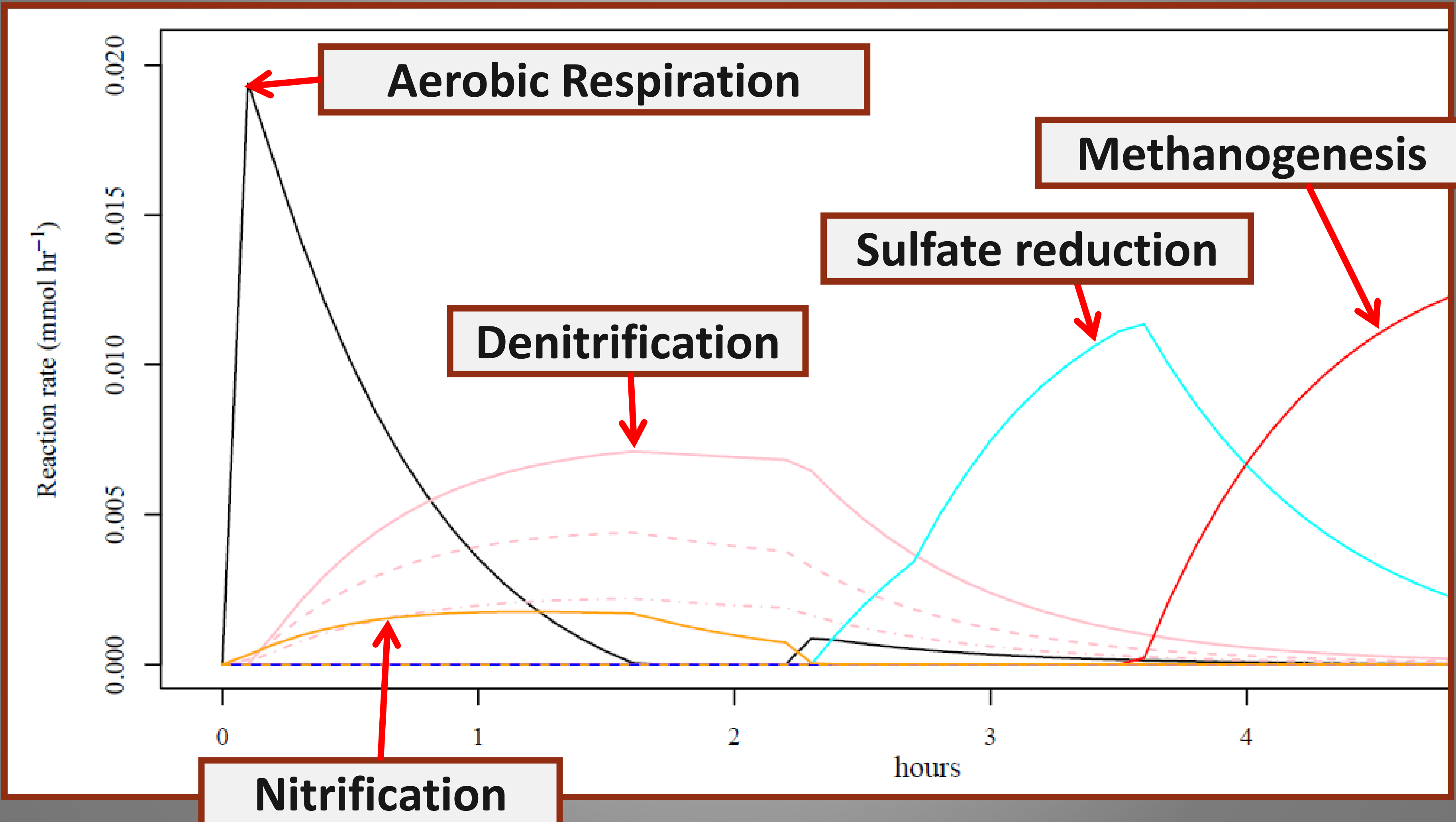
Initial O_2, NO_3^-, SO_4^{-2} = 0.28 mmol L^{-1}

Saturation of O_2 in freshwater at 20˚C

Model demonstration: thermodynamics



Model demonstration: thermodynamics



Model demonstration: stoichiometry

Favor heterotrophic assimilation of DIN

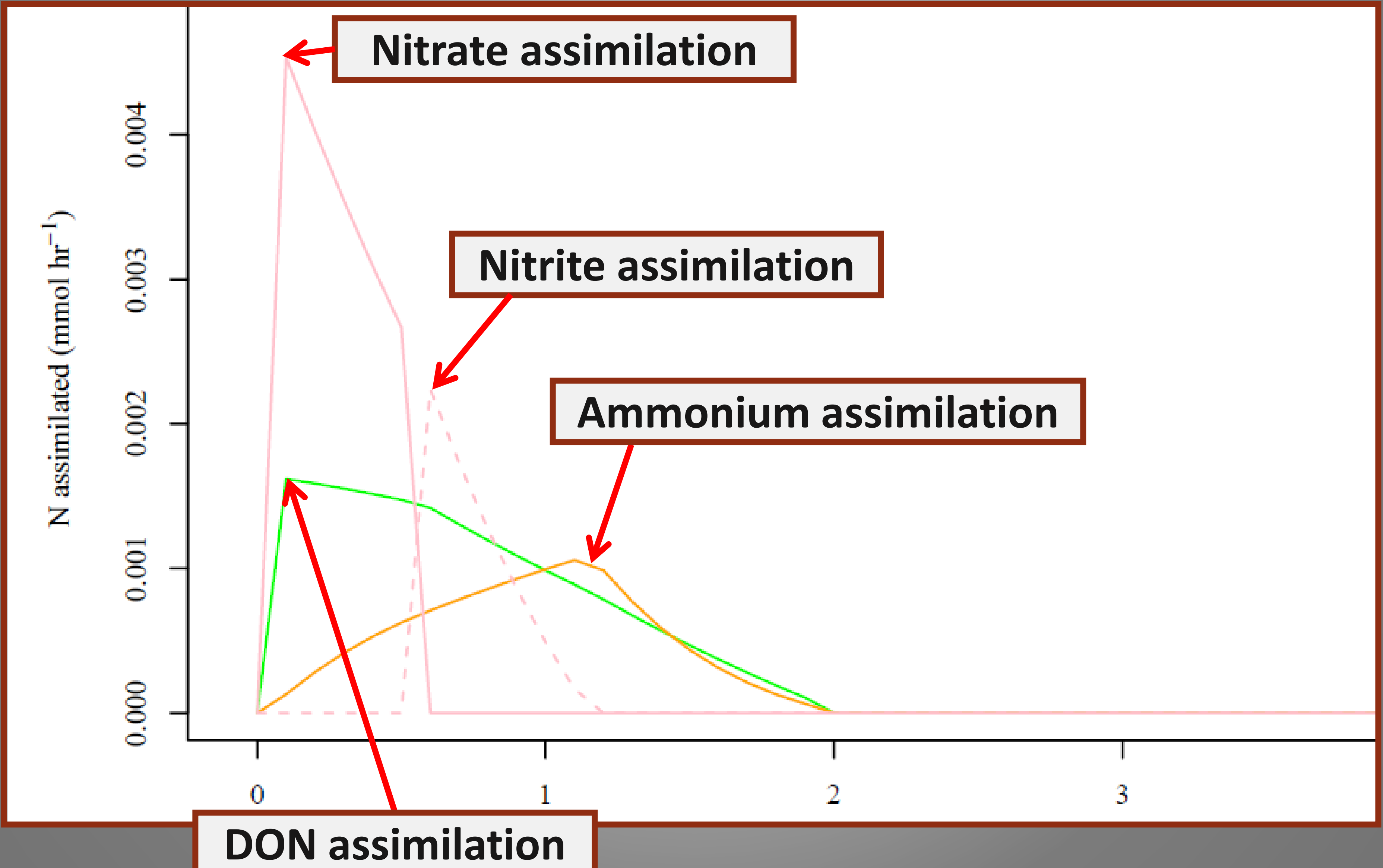
Biomass C:N = 106:16

Redfield Ratio

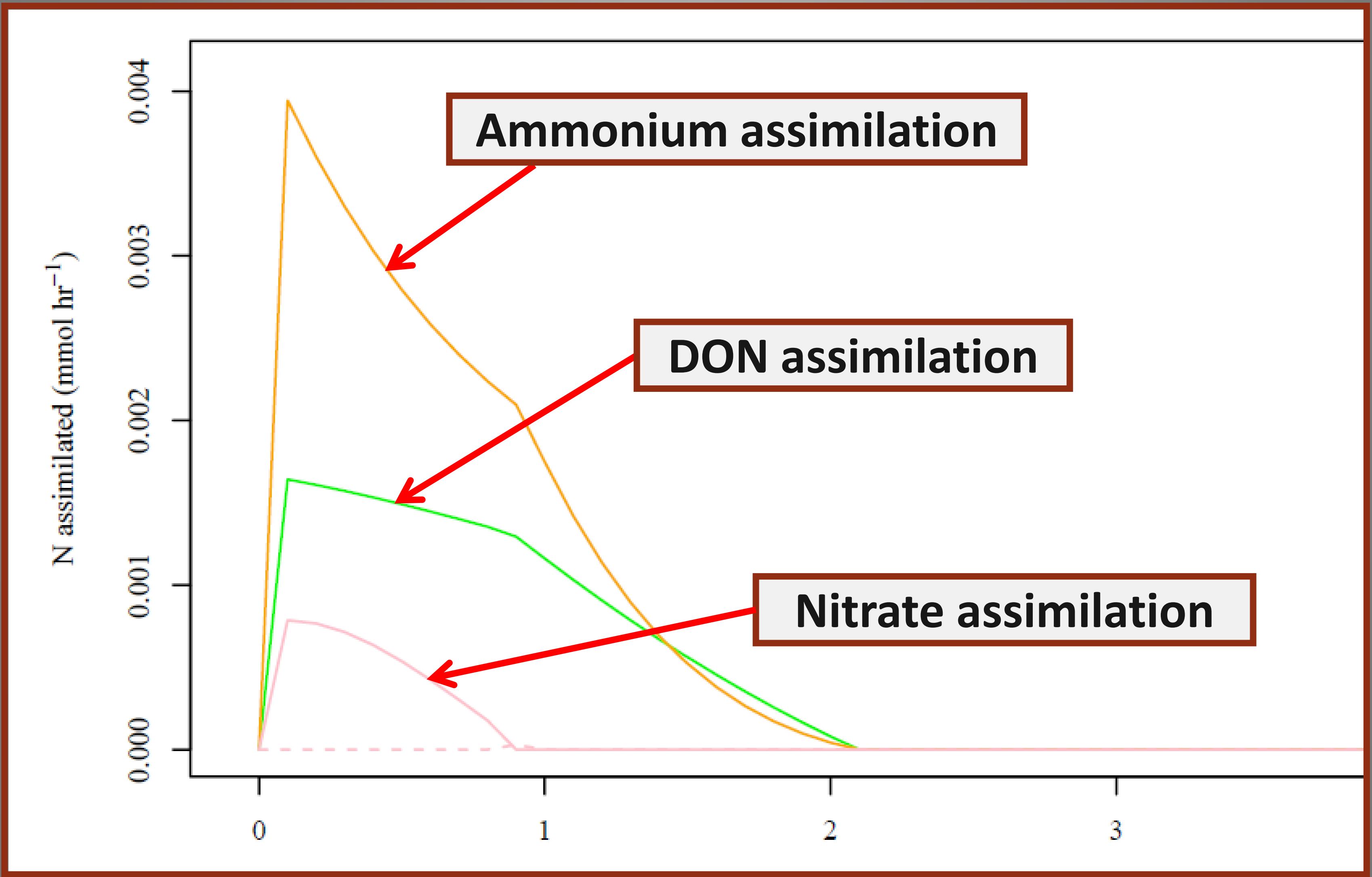
Initial DOC C:N = 106:4

Redfield Ratio x 4

Model demonstration: stoichiometry



Model demonstration: stoichiometry



Concluding remarks

All models are wrong, some are useful

Benchmark in parsimony

Next steps

- Compare with real slurry batch reactor data
- Integrate with hydrologic model