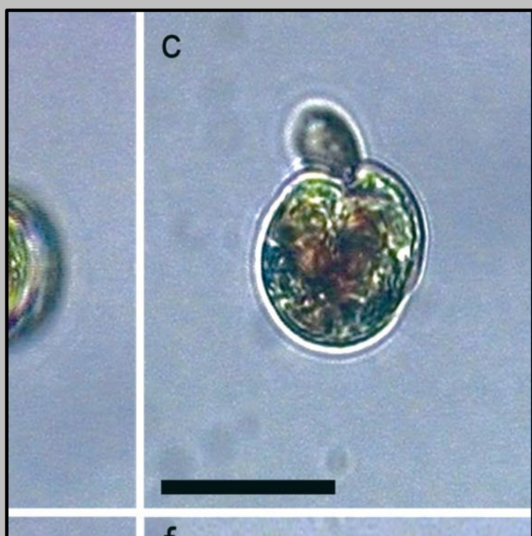
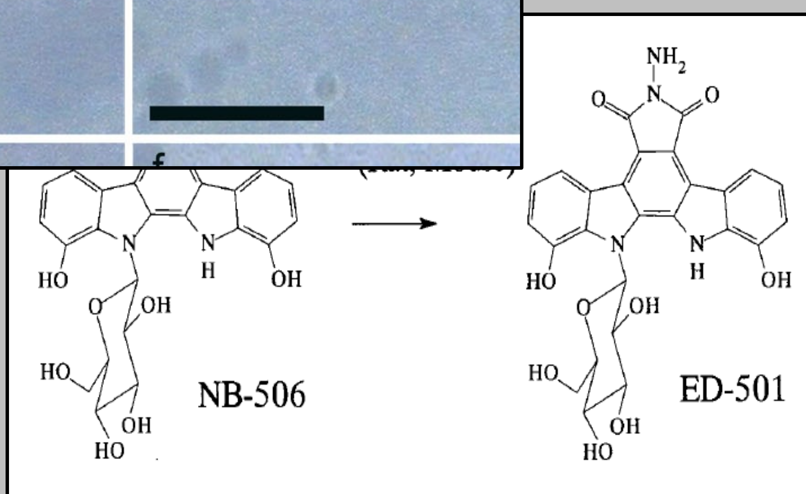
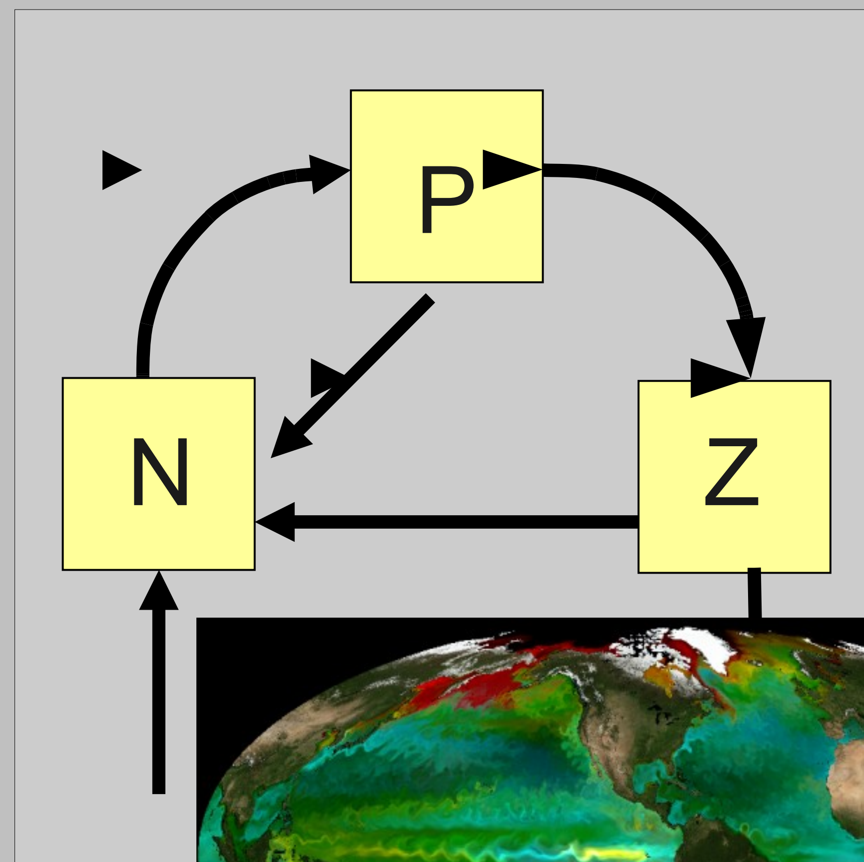
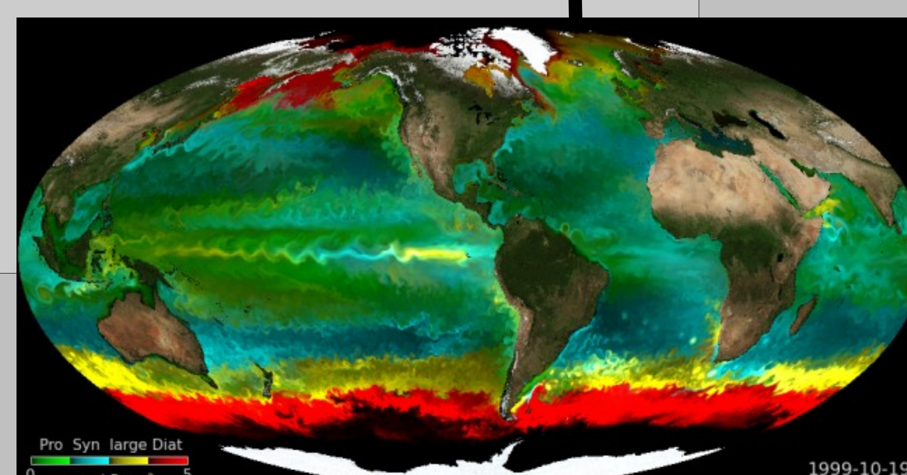
Modeling molecules to ecosystems

Mick Follows (MIT), Ric Williams (Liverpool University)



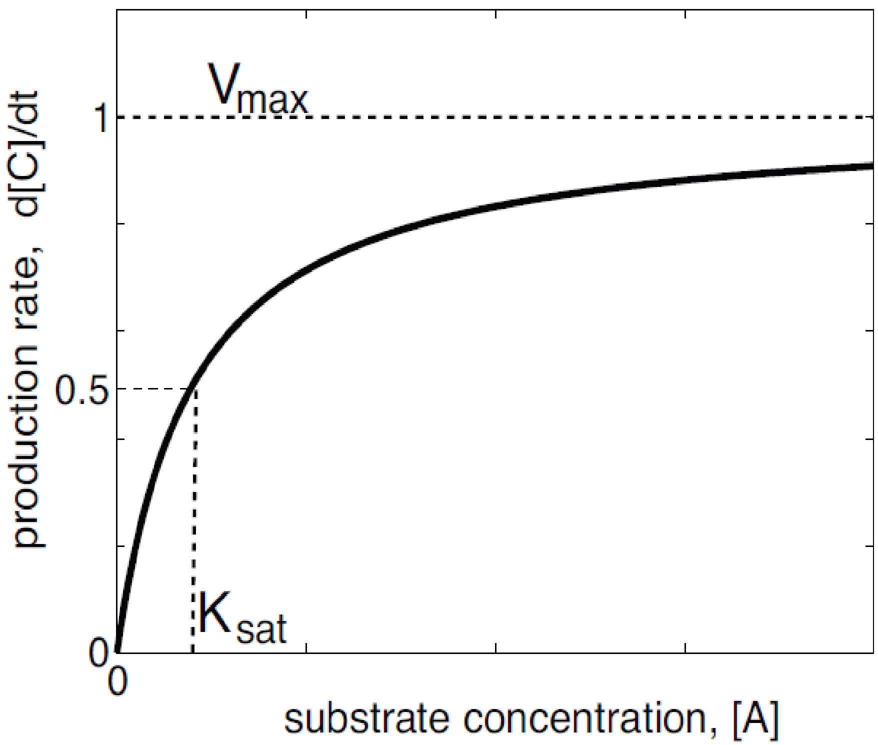






Michaelis-Menten relationship

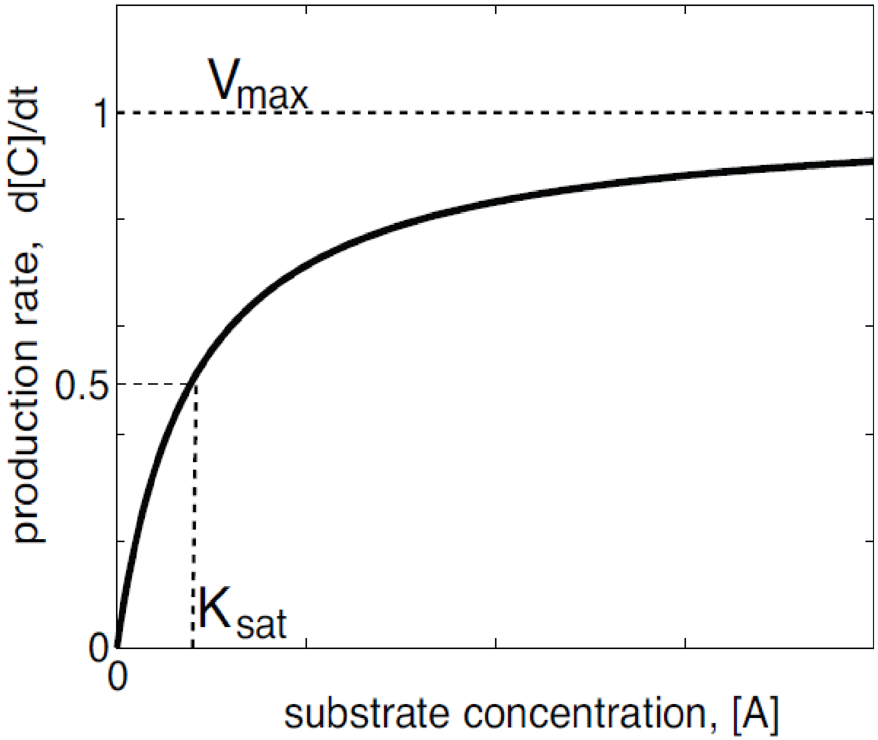
P_C



$$P_C = \frac{d[C]}{dt} = V_{max}\frac{[A]}{K_{sat}+[A]}$$

Michaelis-Menten relationship

P_C

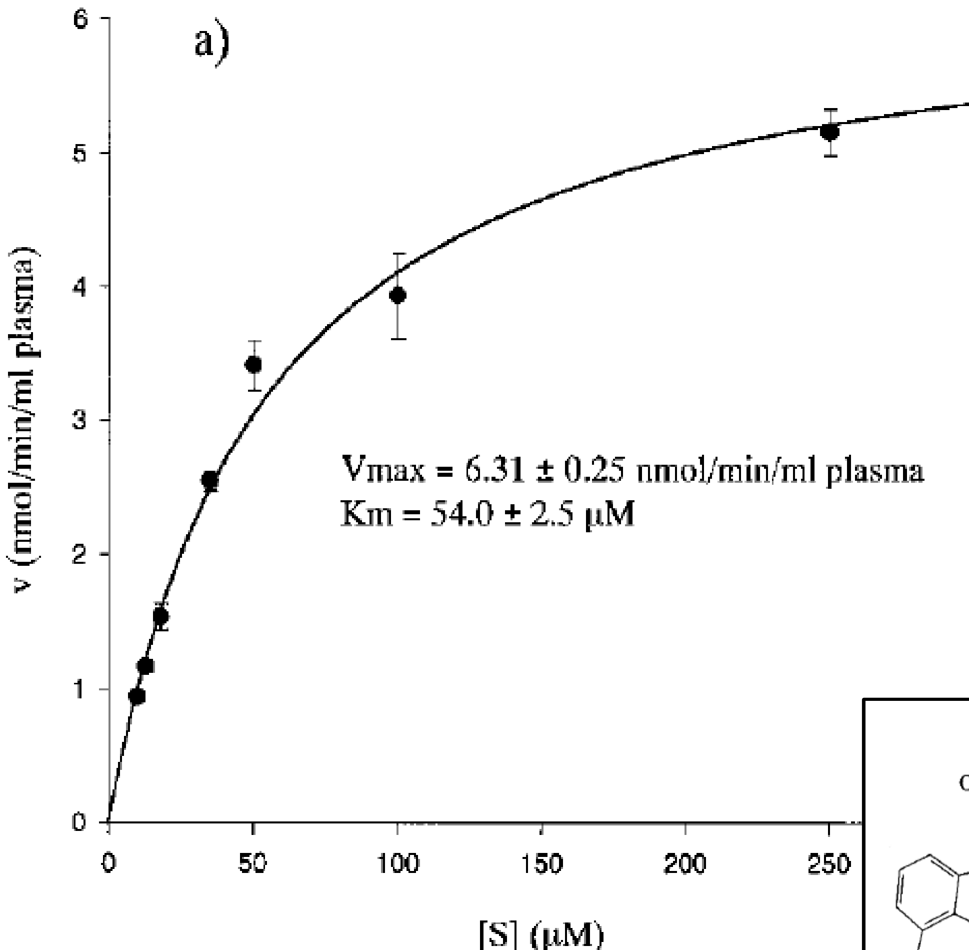


$$P_C = \frac{d[C]}{dt} = V_{max}\frac{[A]}{K_{sat}+[A]}$$

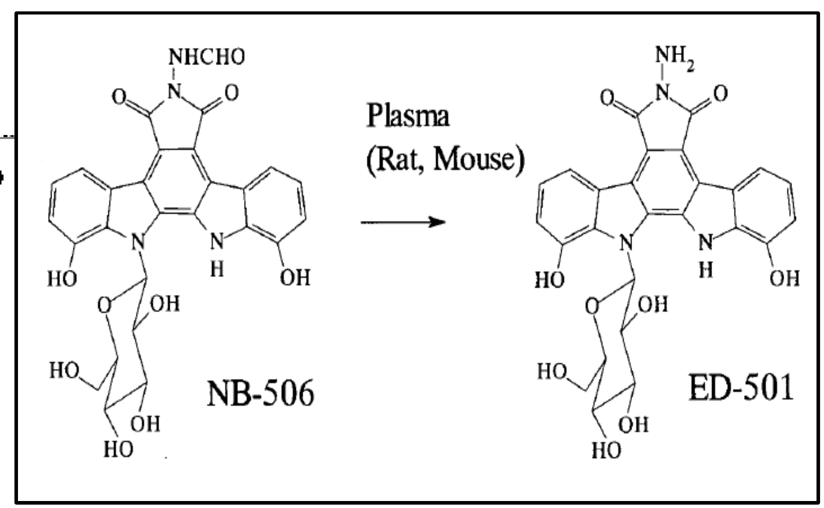
V_{max} = maximum production rate

K_{sat} = half-saturation

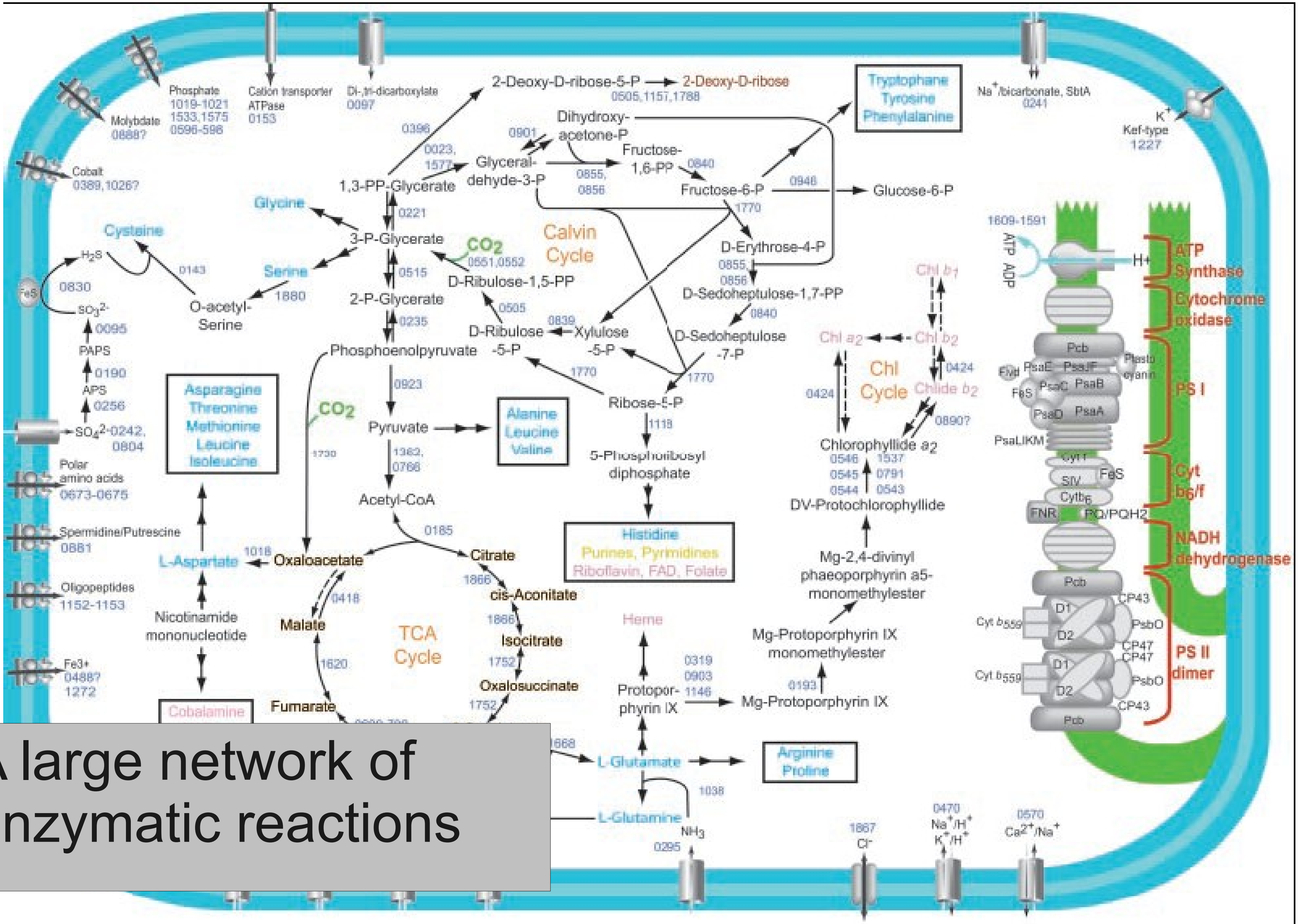
Enzymatic reaction



- Takenaga et al. (1999) *Drug Metabolism and Disposition*, 27, 213
- Enzyme kinetics of conversion of NB-506 to ED-501 in rat plasma

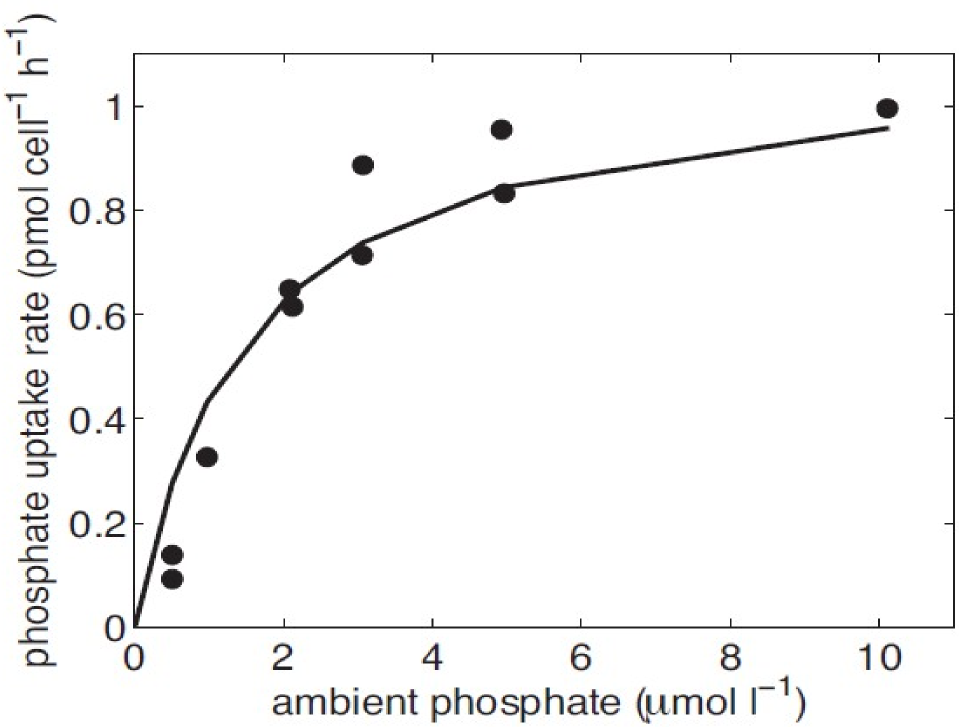


Metabolic pathways of *Prochlorococcus*
Dufresne et al. (2003)



A large network of enzymatic reactions

Phosphate uptake

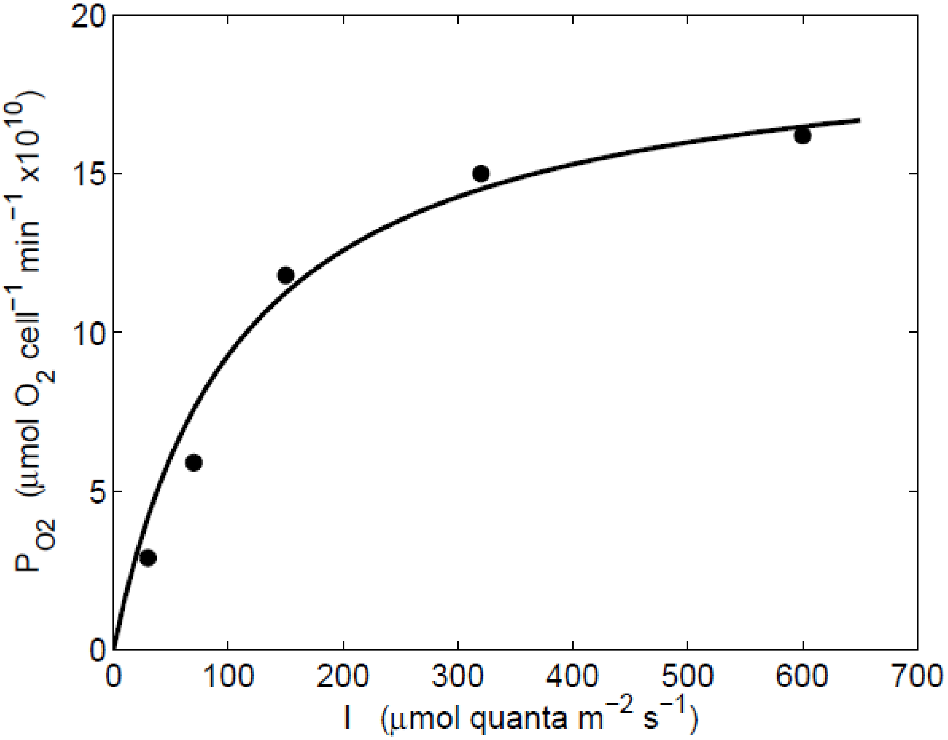


- Phosphate uptake by a laboratory culture of phytoplankton
- Redrawn from Yamamoto and Taruntani (1999)
- Solid line:

$$V = V_{max} \frac{PO_4}{PO_4 + k_{sat}}$$

- V_{max} = 1.1 pmol cell^{-1} hr^{-1}
- K_{sat} = 1.5 μmol l^{-1}

Photosynthesis and irradiance



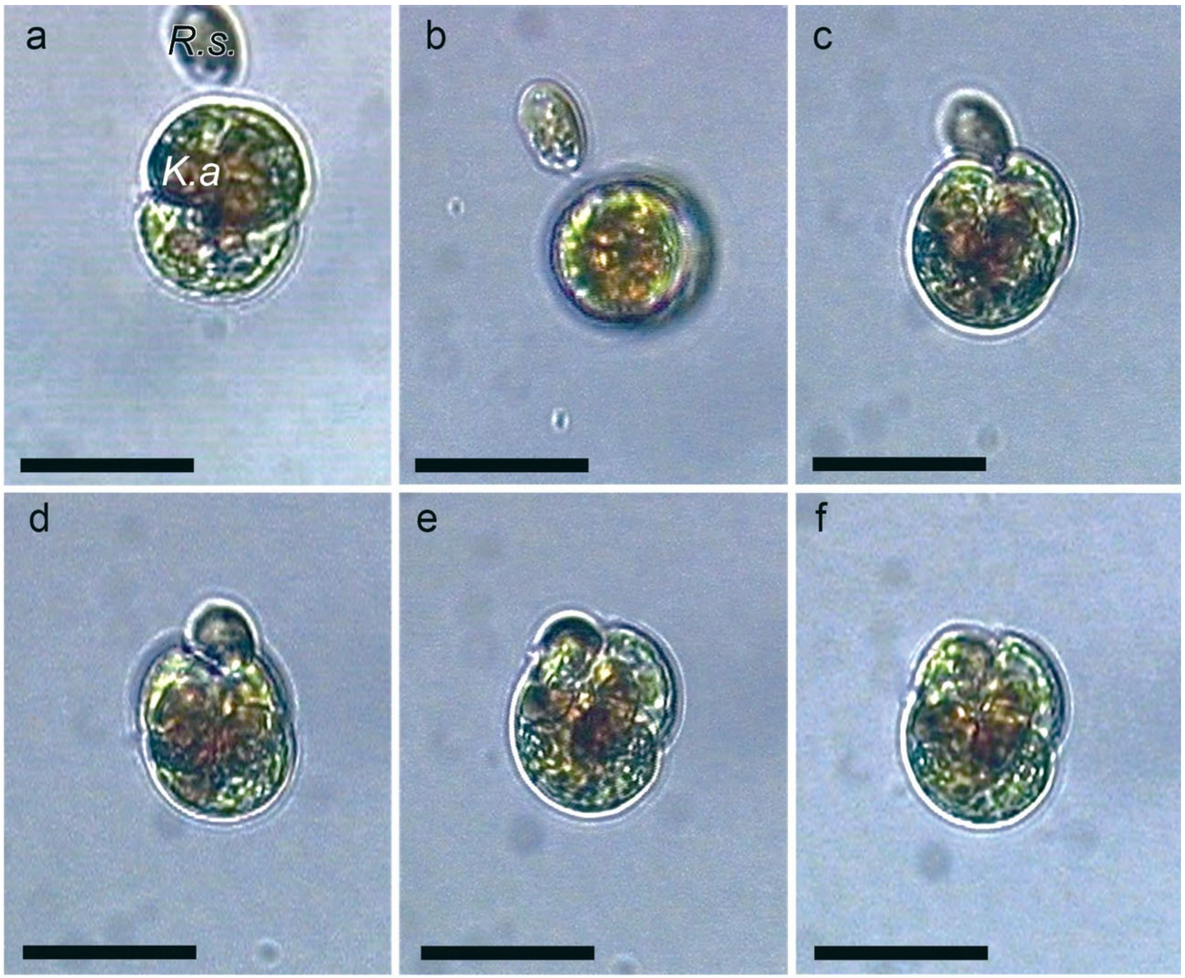
- Falkowski et al. (1985)
- *Isochrysis galbana* in laboratory culture

$$P_{O2} = P_{O2}^{max} \frac{I}{I + k_I}$$

P_{O2}^{max} = 19.5 μmol O2 cell^{-1} min^{-1} x10^{10}

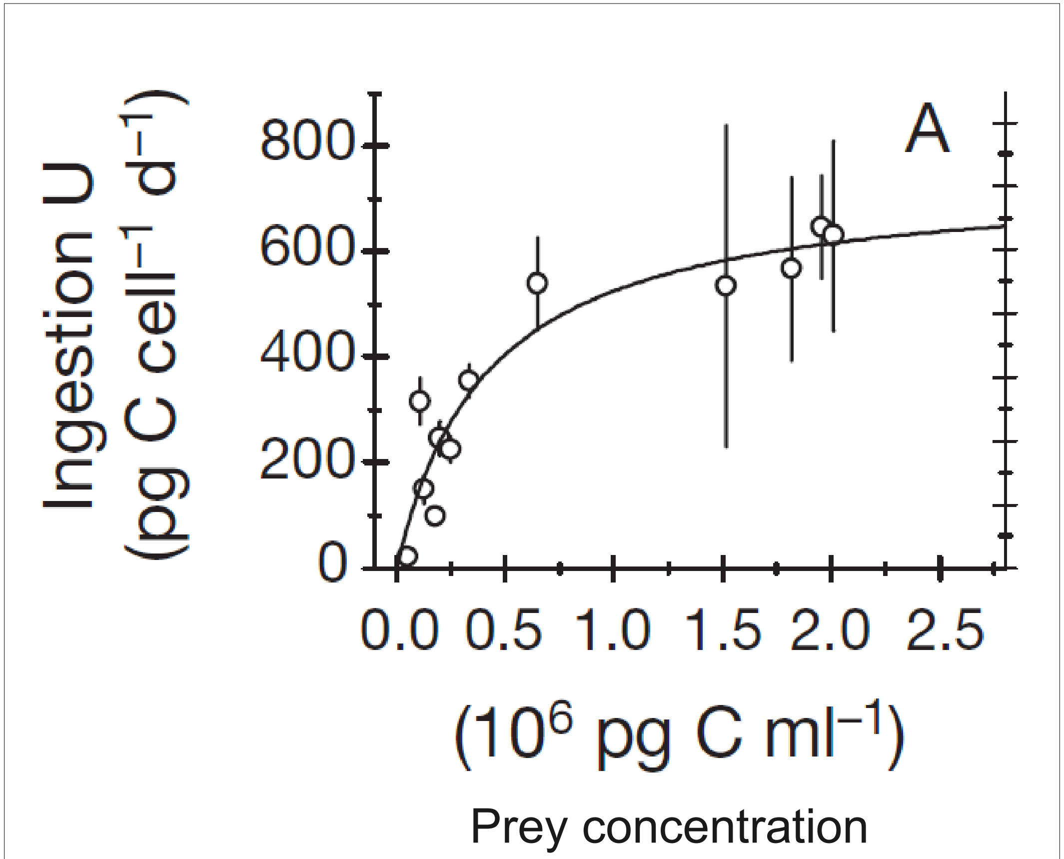
KI = 110.0 μmol quanta m^{-2} s^{-1}

Predation and prey density



- Berge et al. *Aquatic Microbial Ecology*, **50**, 279, (2008)
- Ingestion of phytoplankton *Rhodomonas salina* by dinoflagellate *Karlodinium armiger* in laboratory setting

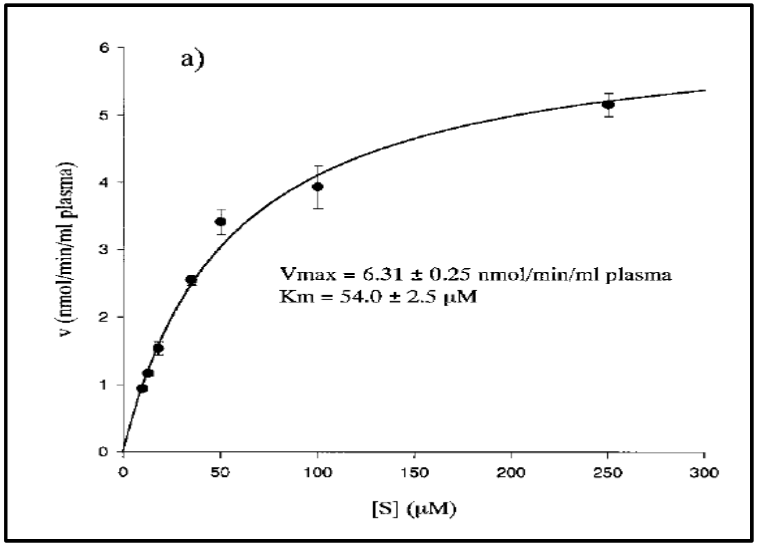
Predation and prey density



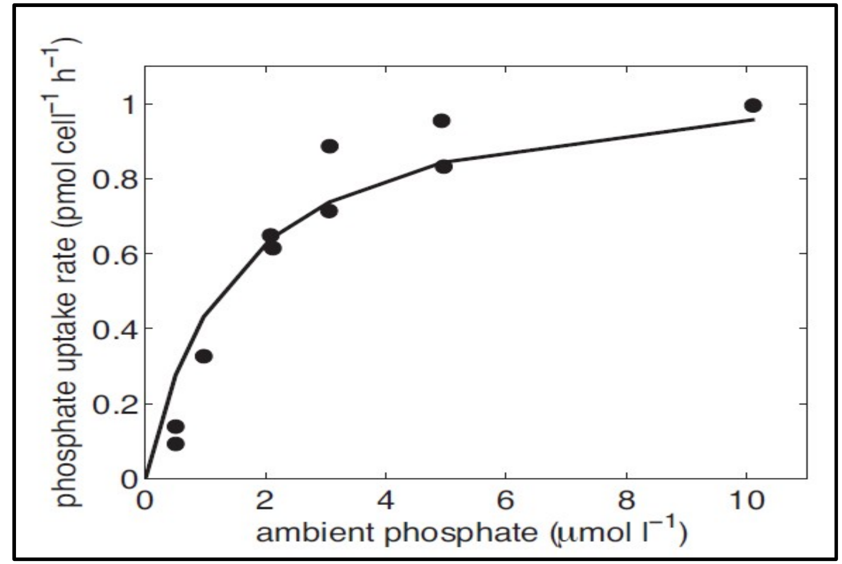
- Berge et al. *Aquatic Microbial Ecology*, **50**, 289 (2008)
- Ingestion rate of phytoplankton *Rhodomonas salina* by dinoflagellate *Karlodinium armiger* in laboratory setting

Why can all be described by the same function?

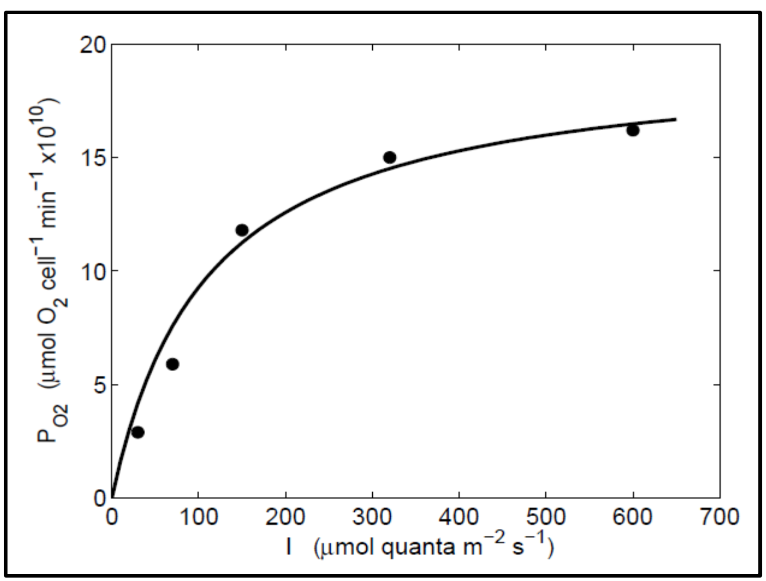
Enzymatic reaction



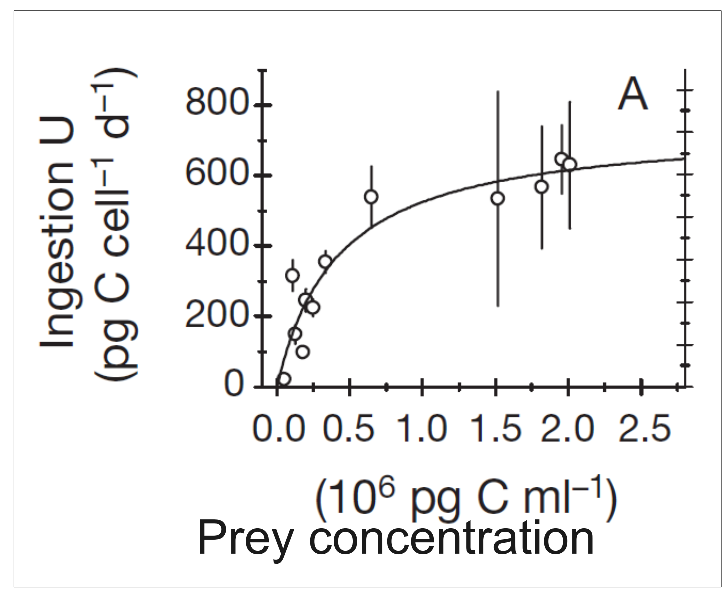
Microbial nutrient uptake



Photosynthesis-irradiance



Predator-prey



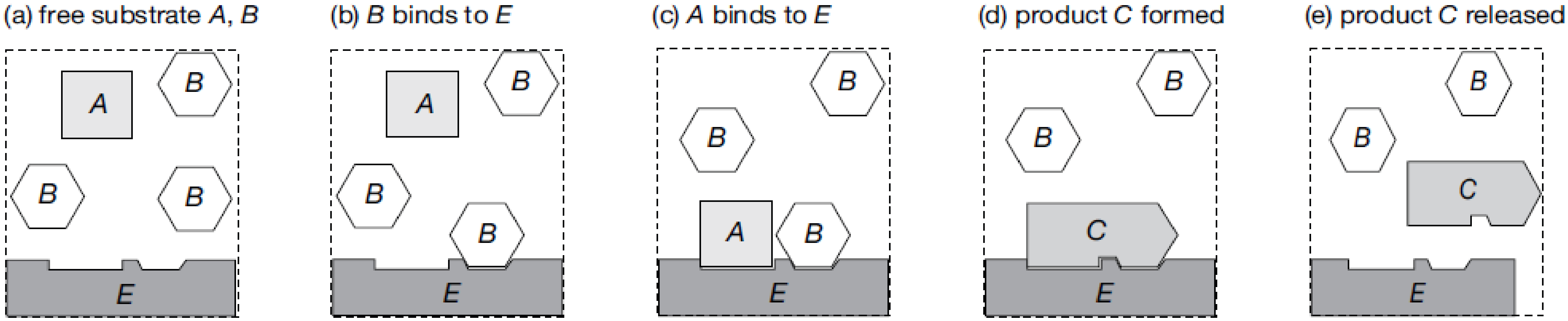
Michaelis-Menten: Enzyme kinetics

Leonor Michaelis and Maud Menten (1913)

Described succinctly by Caperon (1967) posted with course syllabus

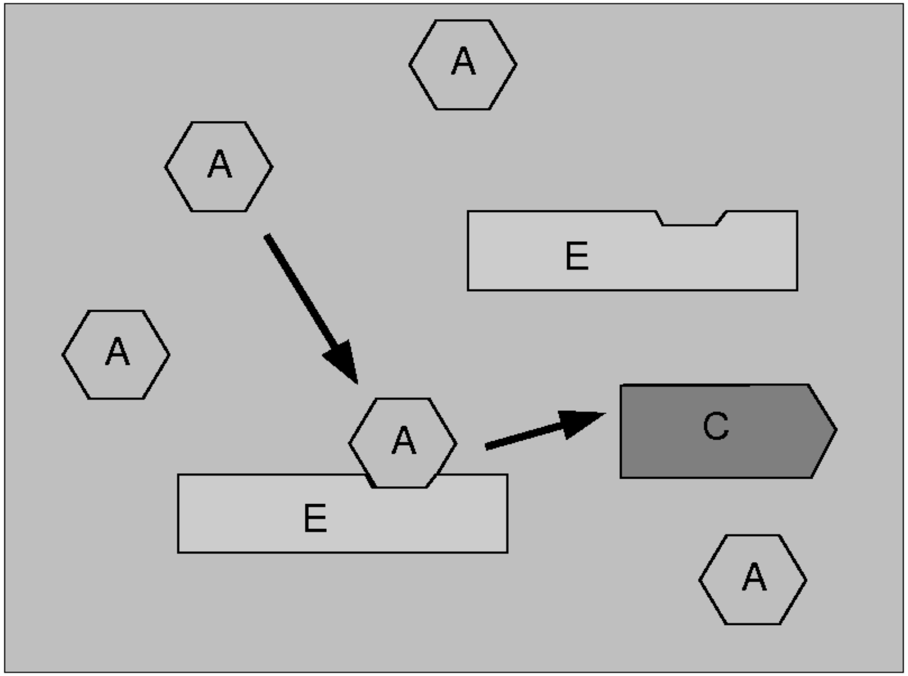
Menten and Michaelis

schematically



Simplest model of enzymatic reaction

$$A + E \rightarrow A \cdot E \rightarrow E + C$$



Simplest model of enzymatic reaction

$$A + E \rightarrow A \cdot E \rightarrow E + C$$

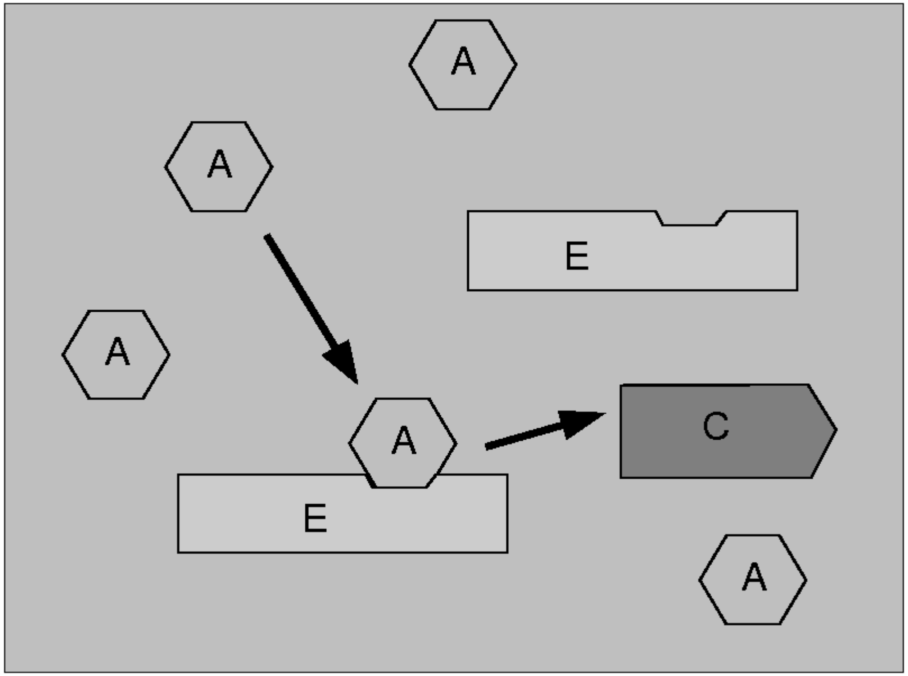
substrate

free enzyme

Substrate-enzyme complex

free enzyme

product



Simplest model of enzymatic reaction

$$A + E \rightarrow A \cdot E \rightarrow E + C$$

substrate

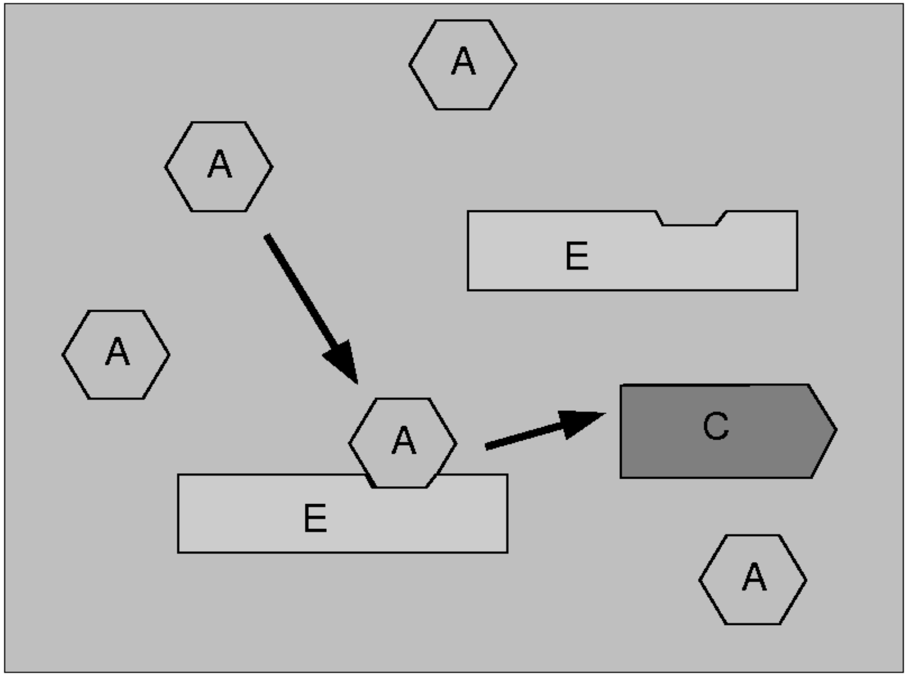
free enzyme

Substrate-enzyme complex

free enzyme

product

[A] = concentration of *A*



Two key relationships

$$[E_T] = [E] + [A \cdot E]$$

Total free complexed

conservation of enzyme

$$\frac{d[A.E]}{dt} = k_E[A][E] - k_H[A \cdot E]$$

rate of change source sink

complex

= rate of production of C, P_c

Two key relationships

$$[E_T] = [E] + [A \cdot E]$$

conservation of enzyme

Total free complexed

mol m^{-3} mol m^{-3} mol m^{-3}

$$\frac{d[A.E]}{dt} = k_E[A][E] - k_H[A \cdot E]$$

complex

rate of change source sink

= rate of production of C, P_c

mol m^{-3} s^{-1} s^{-1} mol m^{-3}

(mol m^{-3} s) $^{-1}$ mol m^{-3} mol m^{-3}

“Encounter” and “handling”

$$[E_T] = [E] + [A \cdot E]$$

conservation of enzyme

$$\frac{d[A.E]}{dt} = k_E[A][E] - k_H[A \cdot E]$$

complex

$1/k_H \quad = \quad \tau_H \quad = \quad$ “handling time” (s)

Time taken for occupied enzyme to catalyze reaction

$1/(k_E[A]) \quad = \quad \tau_E \quad = \quad$ “encounter time” (s)

Time taken until free enzyme encounters molecule of substrate

For completeness, two additional governing equations

$$\frac{d[A]}{dt} = -k_E[A][E]$$

substrate A

$$\frac{d[C]}{dt} = k_H[A \cdot E] = P_C$$

product

Two key relationships

$$[E_T] = [E] + [A \cdot E] \quad (1)$$

$$\frac{d[A.E]}{dt} = k_E[A][E] - k_H[A \cdot E] \quad (2)$$

- Want to describe production rate $P_c = K_H [A.E]$ in terms of substrate concentration $[A]$

Describe production rate in terms of substrate concentration

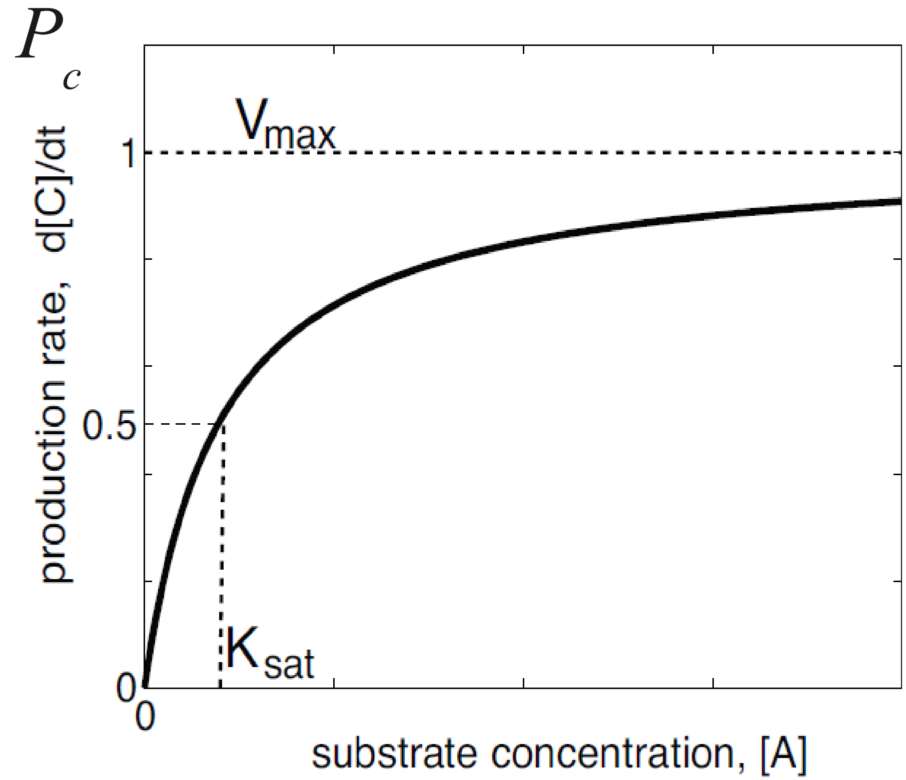
Assuming complex is in “equilibrium” $d[A.E]/dt = 0$

(1) (2) combine to give $$[A \cdot E] = \frac{E_T[A]}{k_H/k_E + [A]}$$

So production rate is

$$\boxed{P_C = \frac{d[C]}{dt} = k_H[E_T]\frac{[A]}{k_H/k_E + [A]}}$$

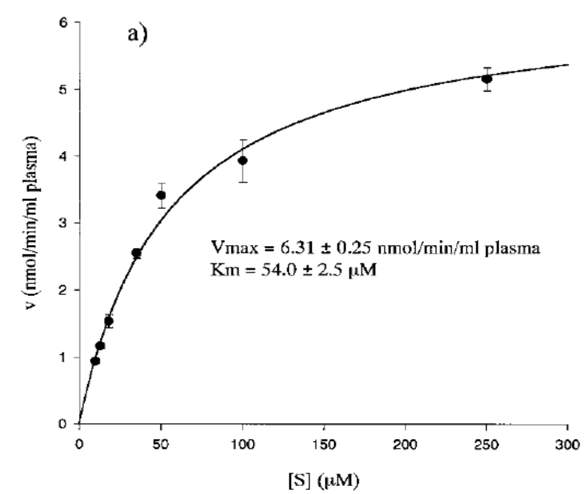
$$P_C = V_{max}\frac{[A]}{K_{sat} + [A]}$$



$$V_{max} = k_H [E_T] \text{ (mol m}^{-3}\text{ s}^{-1}\text{)}$$

Rate of production if all enzymes always fully occupied
Encounter not limiting

$$K_{sat} = k_H / k_E \text{ (mol m}^{-3}\text{)}$$



K_{sat} is harder to interpret mechanistically. However, the slope of the P_c as *[A]* approaches zero is an alternative second parameter which is more easily interpreted:

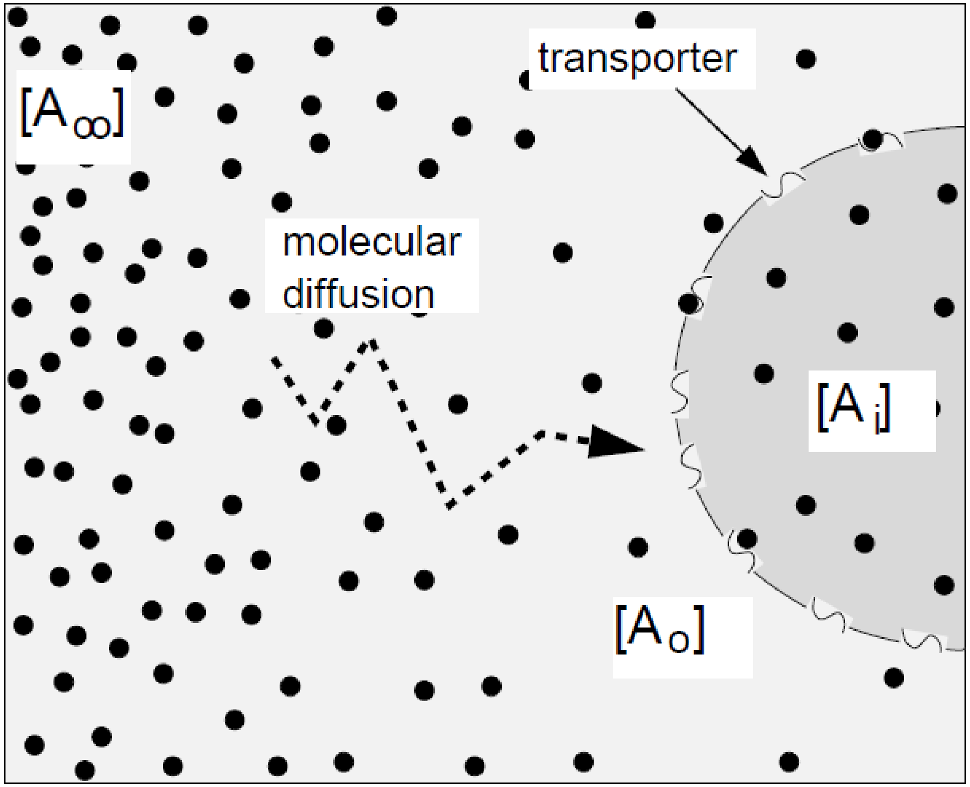
$$P_C = \frac{d[C]}{dt} = k_H[E_T]\frac{[A]}{k_H/k_E + [A]}$$

Differentiating the above relationship with respect to *[A]* and taking the limit *[A]* → *0* leads to

$$\alpha = \frac{dP_C}{dA}([A] \to 0) = k_E[E_T]$$

This is the "affinity" or "clearance rate". It measures the maximum encounter rate – the rate at which substrate molecules are captured if all of the enzymes are always free. (i.e. extreme encounter limited situation).

Nutrient acquisition



- Transporter mediated uptake at cell wall
- Down-gradient diffusion towards cell through molecular boundary layer

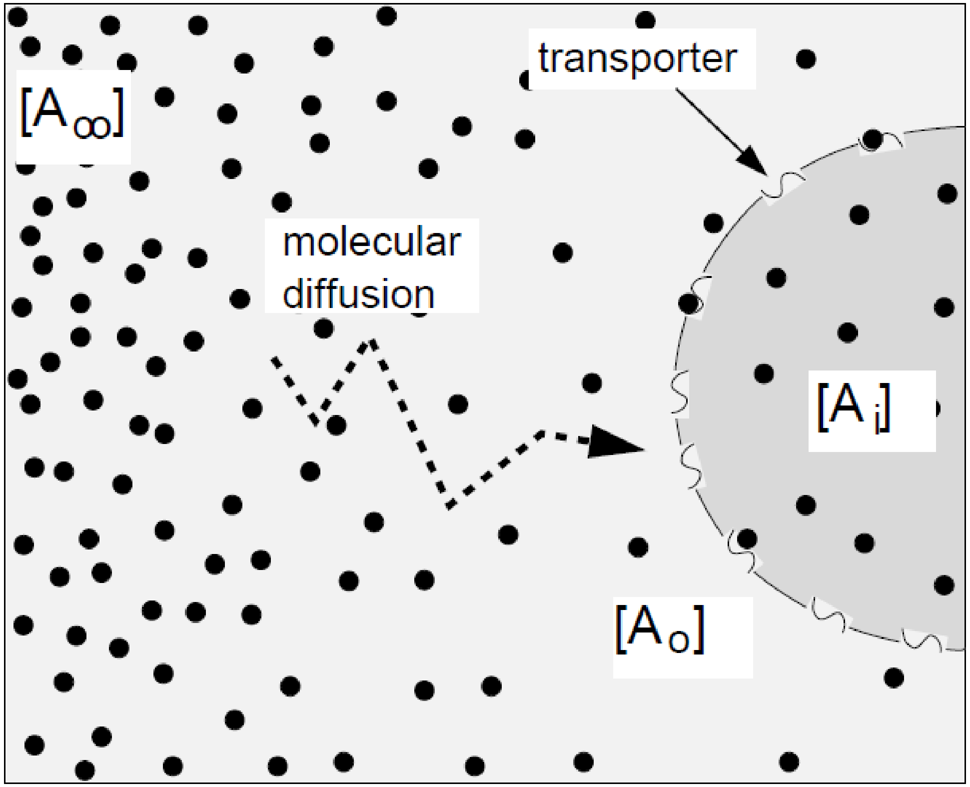
- Munk and Riley, Pasciak and Gavis, Armstrong,...

$[A_o]$ = nutrient concentration just outside cell wall

$[A_\infty]$ = ambient nutrient concentration in medium

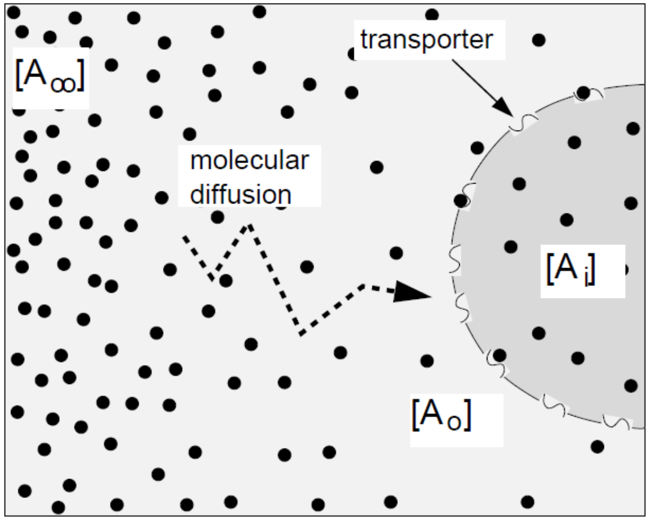
$[A_i]$ = interior concentration of nutrient

Nutrient acquisition



- Want to know rate of uptake (rate of increase of $[A_i]$) as a function of concentration in medium $[A_\infty]$

Treat transfer across cell wall by transporter like enzymatic reaction



$$A_o + E \rightarrow A.E \rightarrow A_i + E$$

$$[E_T] = [E] + [A \cdot E]$$

conservation of transporters

Total free occupied

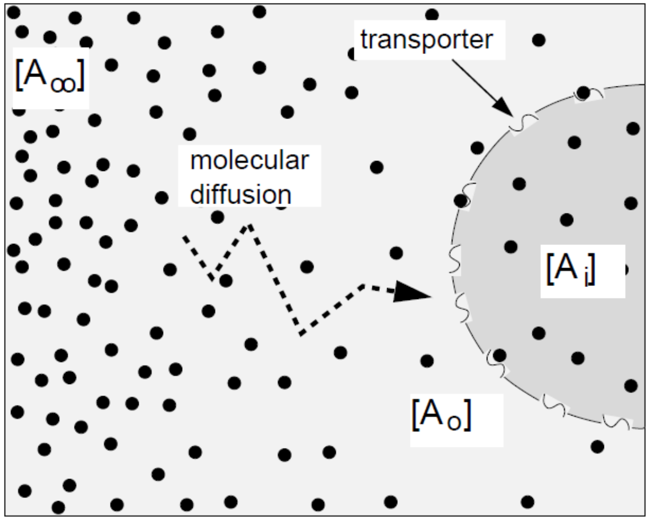
$$\frac{d[A.E]}{dt} = k_E[A_o][E] - k_H[A \cdot E]$$

occupied transporters

rate of change encounter nutrient transfer into cell

N.B. [ ] now denotes surface area density and units of KE are thus $(\text{mol m}^{-2}\text{ s})^{-1}$

Treat transfer across cell wall by transporter like enzymatic reaction

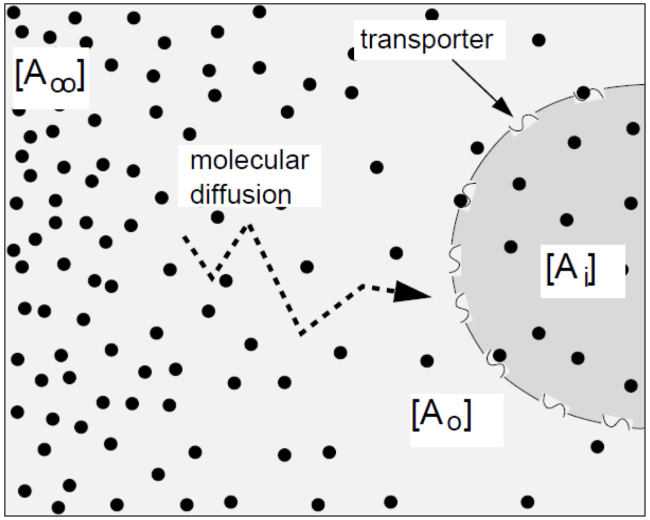


Assume transporters in "equilibrium" $d[A.E]/dt = 0$

Following above

$$V = \text{uptake} = k_H[E_T]\frac{[A_o]}{k_H/k_E + [A_o]}$$

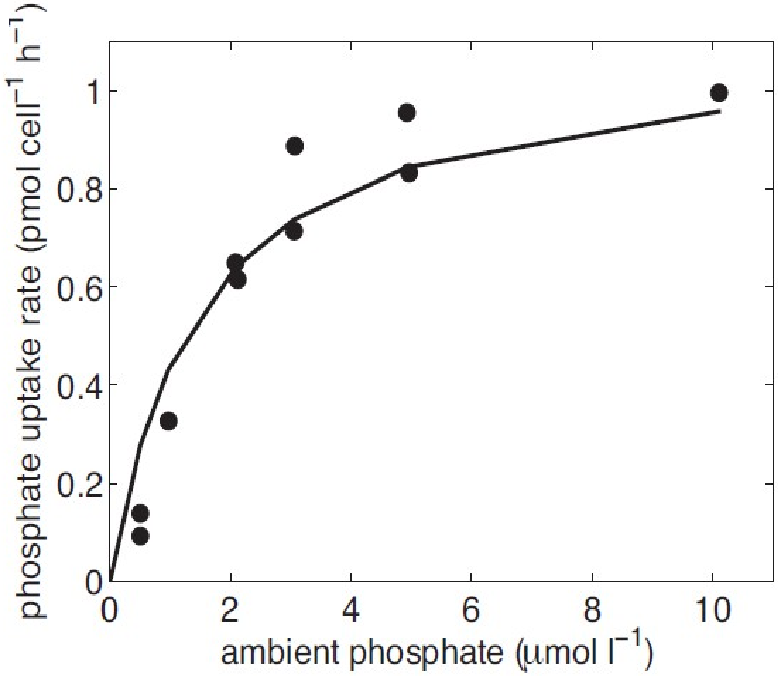
- If diffusion towards cell rapid relative to uptake across cell wall, $[A_o] \sim [A_\infty]$
- Case when transporter across cell wall is limiting



$$V \sim k_H [E_T] \frac{[A_\infty]}{k_H/k_E + [A_\infty]}$$

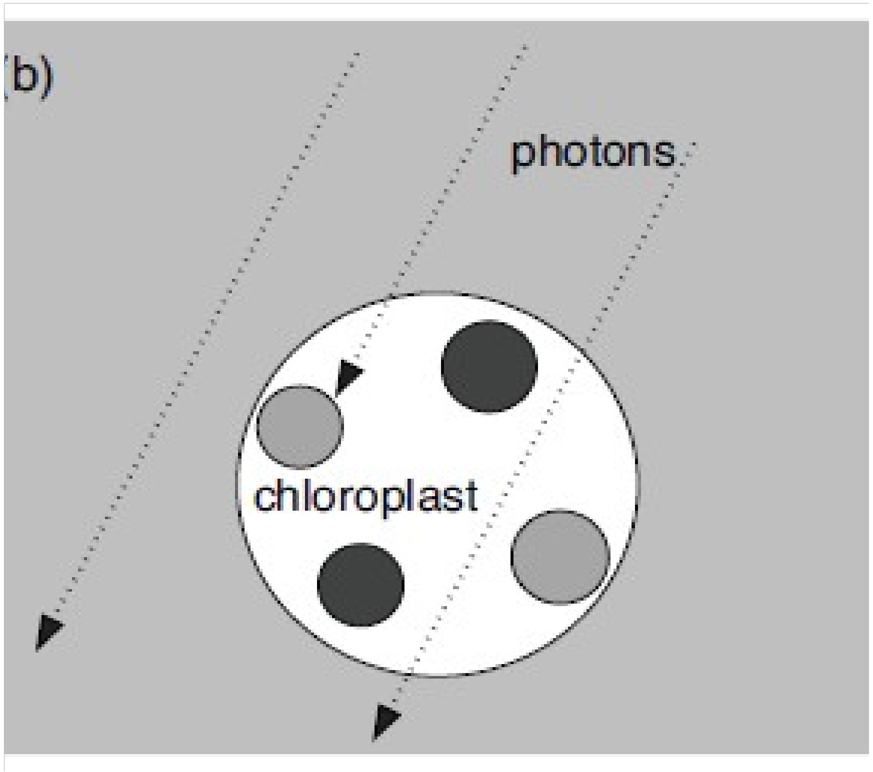
$$V_{max} = k_H [E_T] \qquad K_{sat} = k_H / k_E$$

- Maximum uptake depends on total density of transporters *[E_T]*
- ...acclimation.

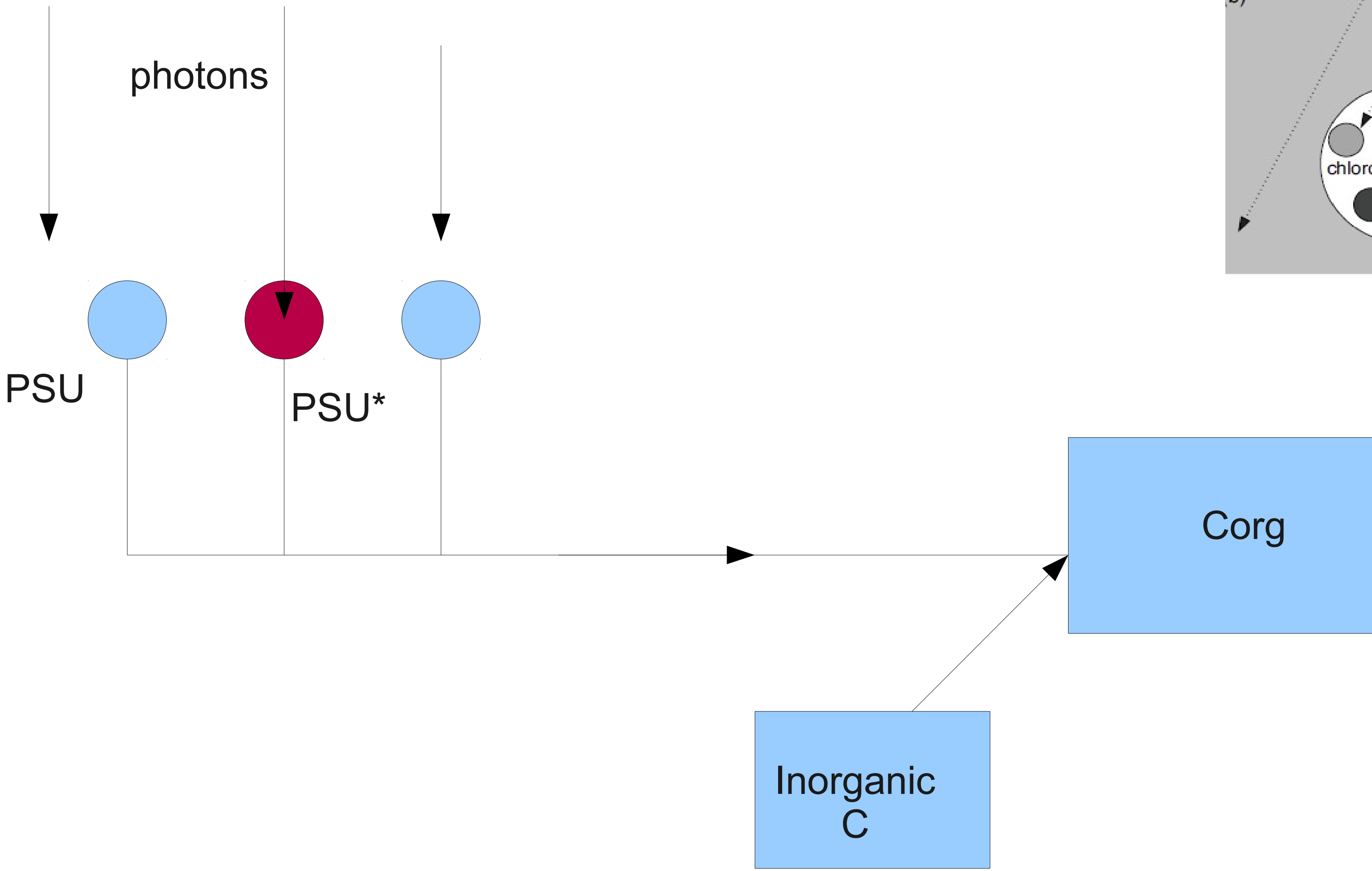


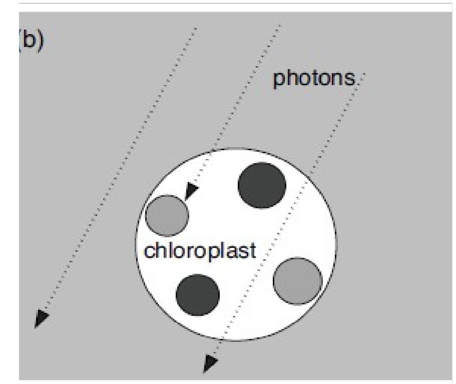
See Armstrong (2008), Karp-Boss et al (1996)

Photosynthesis-irradiance



Photosynthesis-irradiance





$$PSU + photons \rightarrow PSU* \rightarrow PSU + C_{org}$$

$$PSU + photons \rightarrow PSU* \rightarrow PSU + C_{org}$$

Two key relationships:

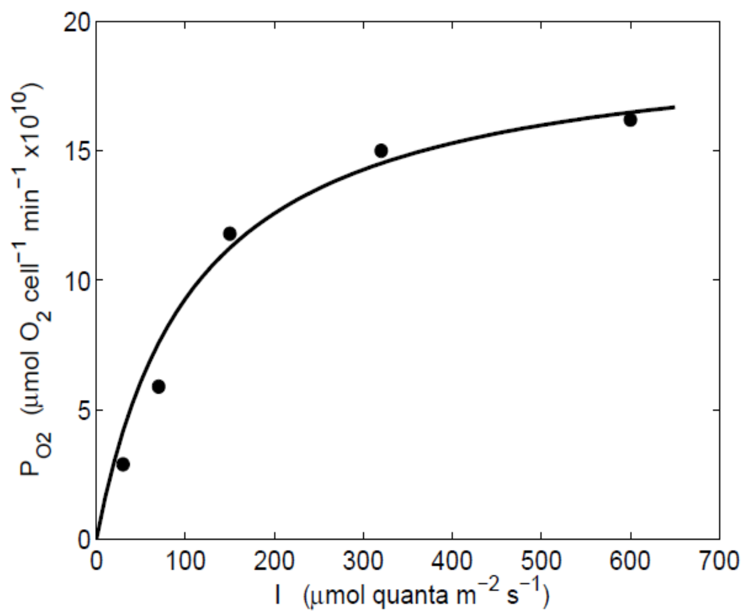
$$PSU_T = PSU + PSU*$$

$$\frac{dPSU*}{dt} = \sigma \; I \; PSU - k_H PSU* \;\; \sim \;\; 0$$

Photosynthesis - irradiance

$$\mathrm{Photosynthesis} = \mathrm{k_H}\ \mathrm{PSU_T} \frac{\mathrm{I}}{\mathrm{k_H}/\sigma + \mathrm{I}}$$

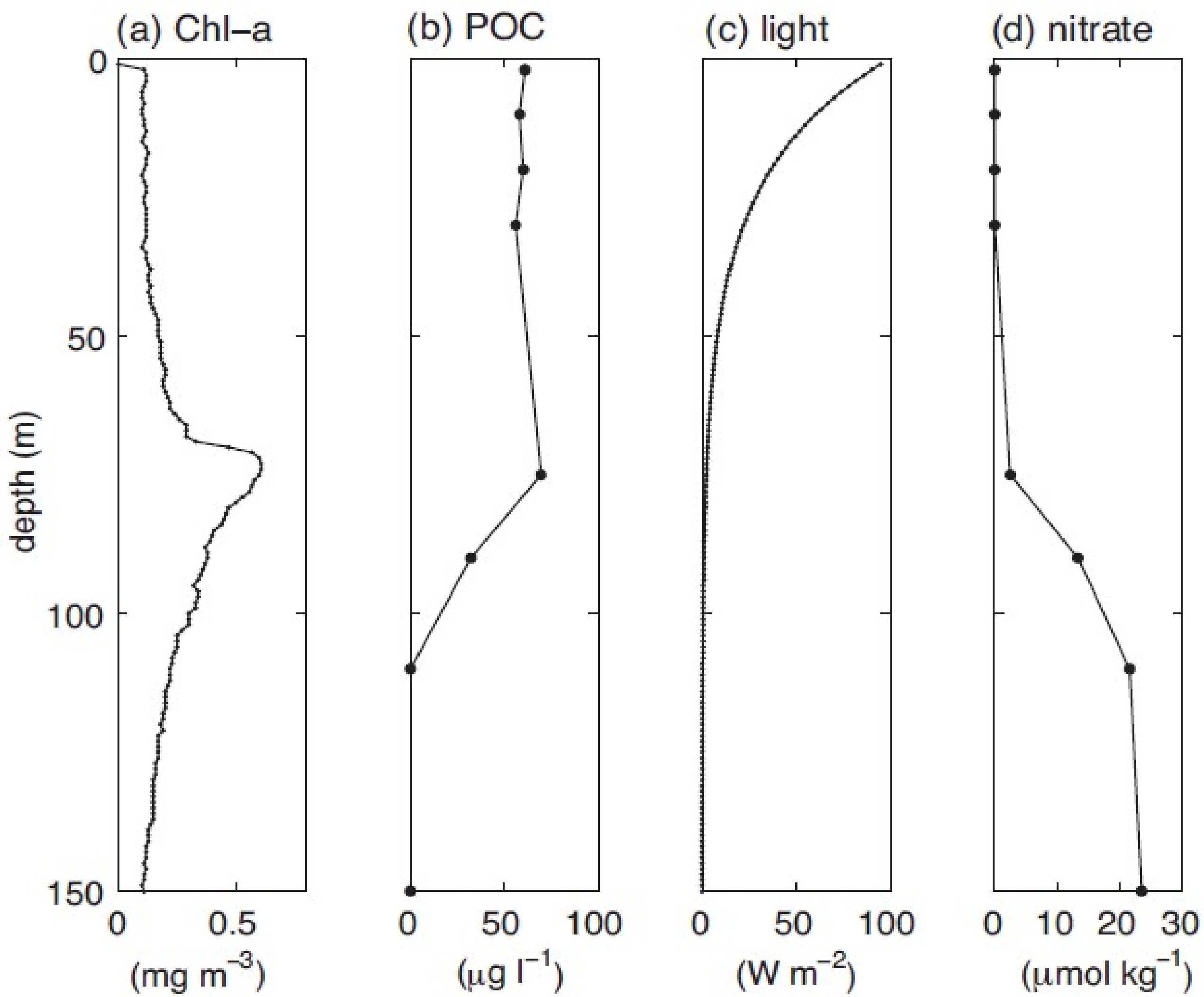
Max rate of photosynthesis = $K_H\, PSU_T$



Proportional to amount of pigment and "handling time"

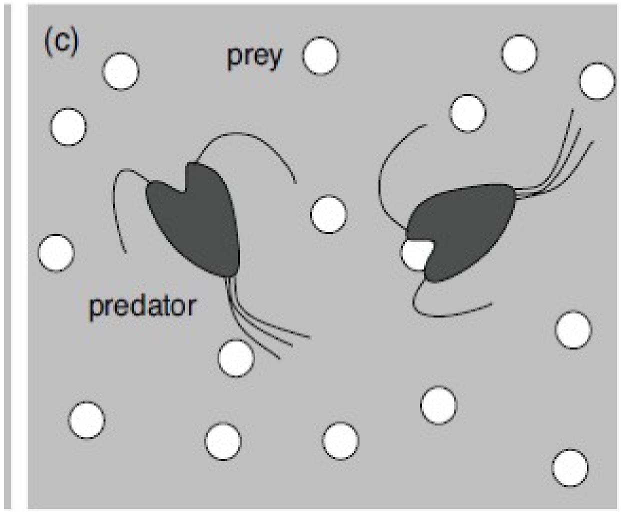
Acclimation by changing pigment concentration or downstream efficiency of utilizing captured energy

Acclimation of pigments in nature



- Data from Anna Hickman
- Atlantic Meridional Transect 15, 2.5°N, 24.5°W

Predator-Prey Interactions



predator + prey → occupied predator → predator

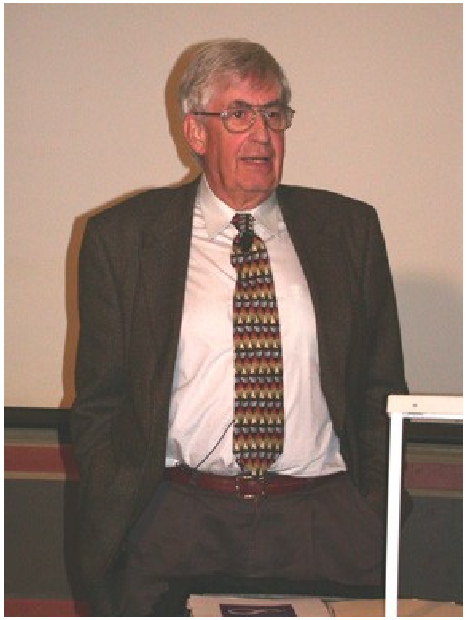
$$\text{Predation rate} = k_H \, Z_T \frac{P}{k_H/K_E + P}$$

Z_T = total predator density

P=prey density

Holling type II

C.S. Holling (1959)



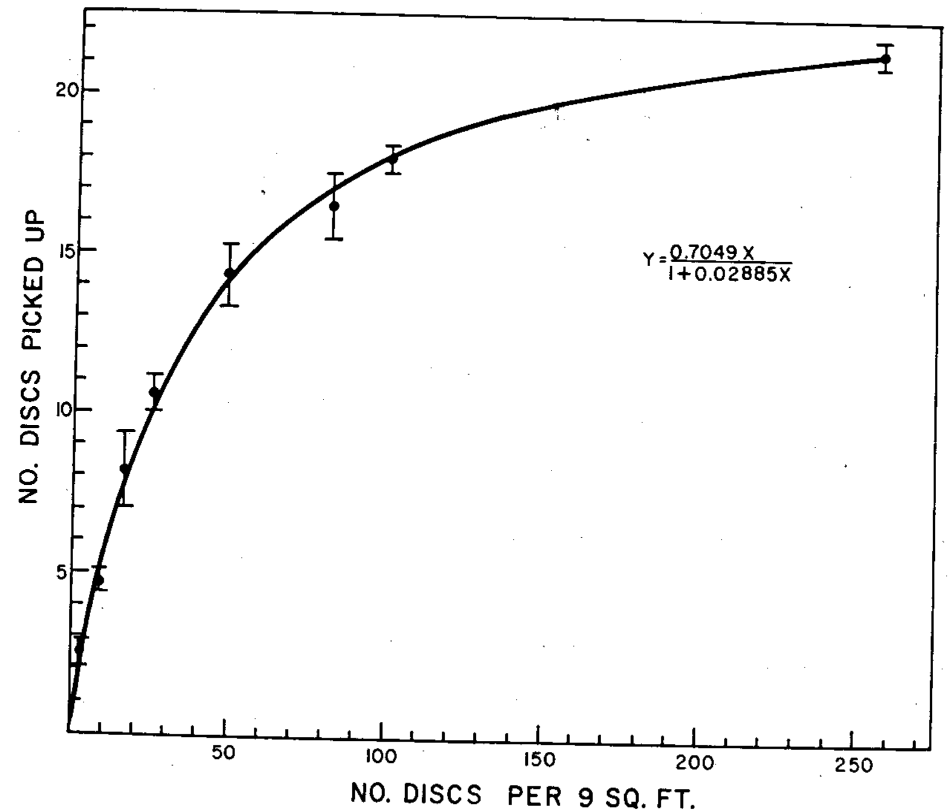
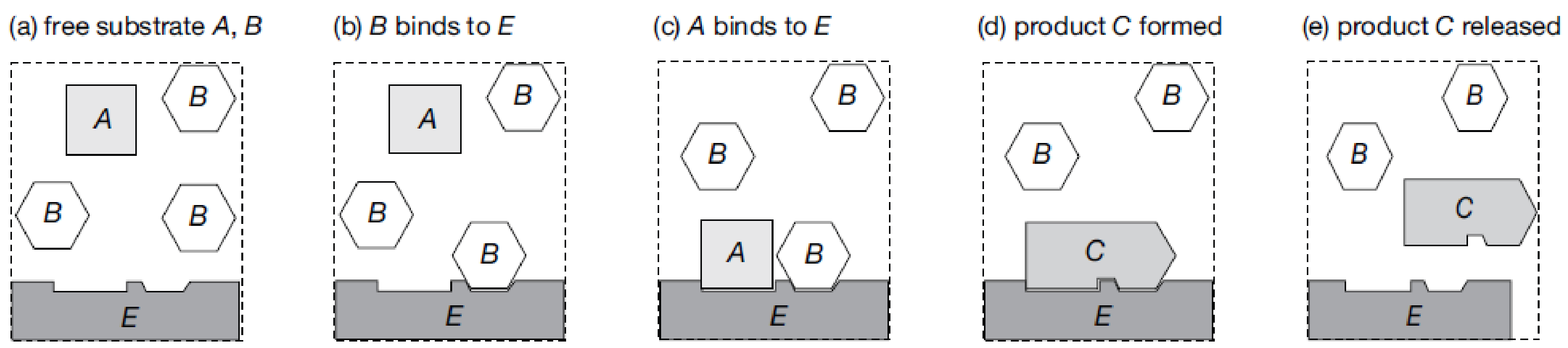
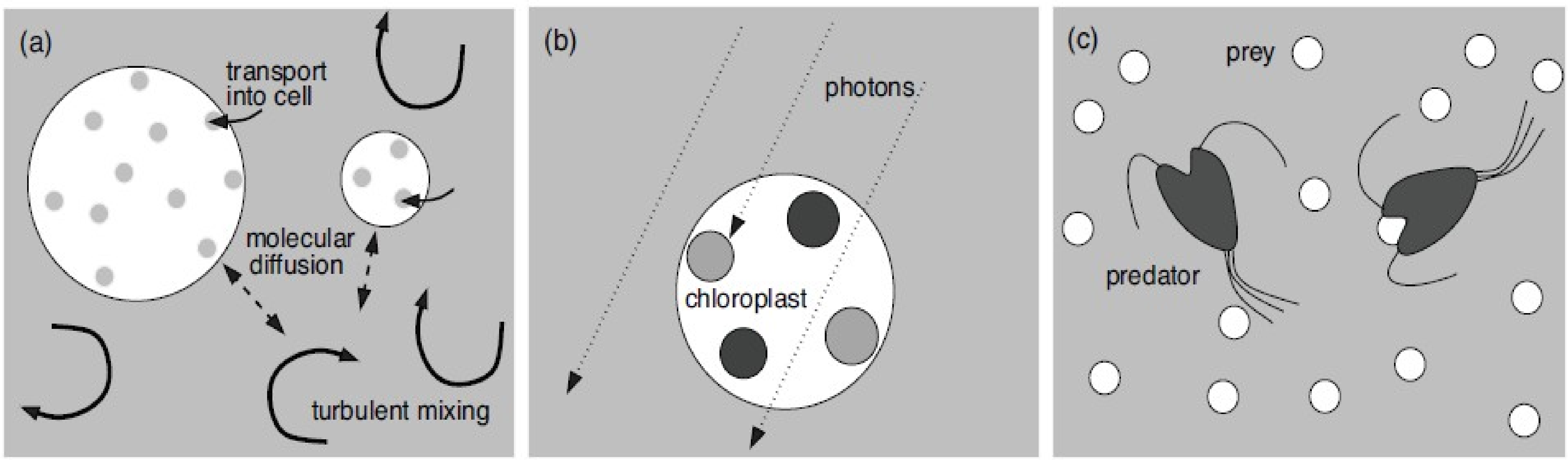


Fig. 1. Functional response of a subject searching for sandpaper discs by touch. (Averages ± 2 S.E. of 8 replicates.)

Holling II function

Two-stage processes





Summary

- Common functional form between “production rate” and “substrate concentration:
    - enzymatic reactions
    - resource acquisition by individuals
    - community interactions and ecosystem-dynamics
- All can be modeled simply and transparently as “two-stage” process