Modelling nitrogen- and light-limited growth of phytoplankton :

Qualitative study and validation of the BioLOV model

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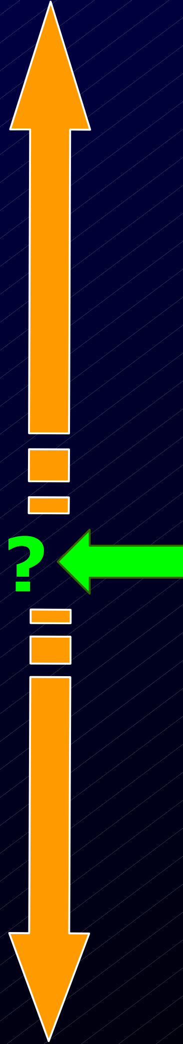
State of the art in Modelling Autotrophic Growth

Simple representations of limited algal growth

→ Too simple to be realistic but integrable into ecosystem or hydrodynamical model

Reference	Number of State variable	Number of parameters	Limitations
Monod, 1956	2	3+	nutrient (but possible $\mu=f(i)$)
Droop, 1968	3	5+	nutrient (but possible $\mu=f(i)$)
Geider *et al.* , 1998	3	12	Light, nitrate, temperature
Zonneveld, 1998	5	14	Light, nutrients
Flynn, 2001	13	55	Light, multinutrients temperature



Complex physiological models

→ Too complex to be validated (lack of data) and integrated into bigger systems

Toward a new model

BioLOV should be a compromise between ...

- the need of simplicity to be integrable into ecosystem or hydrodynamical models.

- the need of detailed algal physiological processes to give accurate carbon fluxes under fluctuating forcings.

Toward a new model

→ *BioLOV should have a simple mathematical formulation with a limited number of parameters.*

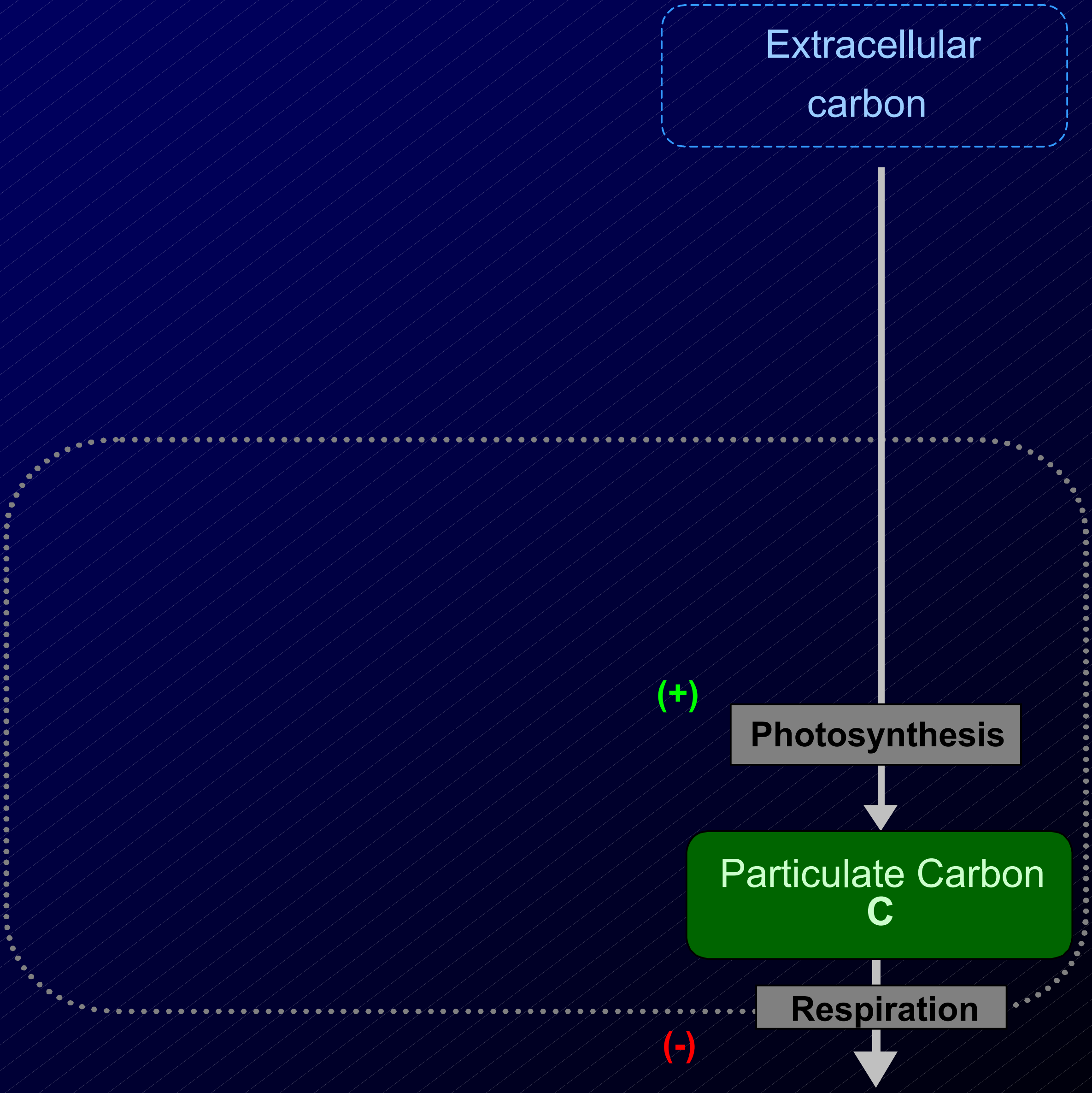
→ *State variables should represent (easily) mesurable algal caracteristics.*

→ *The model should represent "in-water" concentrations instead of cell concentrations.*

→ *The model must respect qualitatively experimental facts.*
(e.g. expected increase or decrease of an output for a change of light or dilution).

Model structure

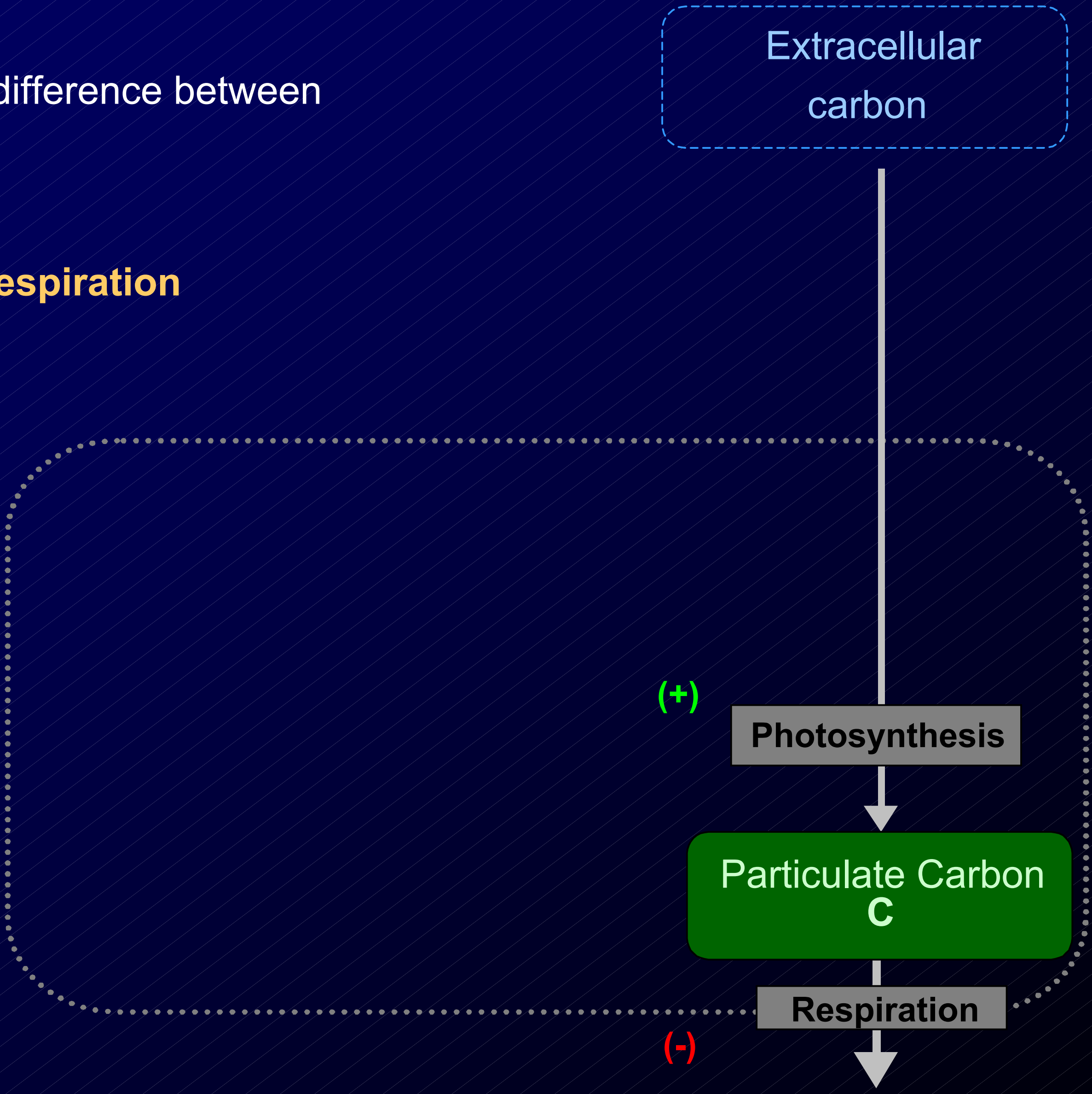
Hypotheses and formulations : Carbon



Hypotheses and formulations : Carbon

-Carbon variation is the result of the difference between photosynthesis and respiration.

$$\frac{dC}{dt} = \text{Photosynthesis} - \text{Respiration}$$



Hypotheses and formulations : Carbon

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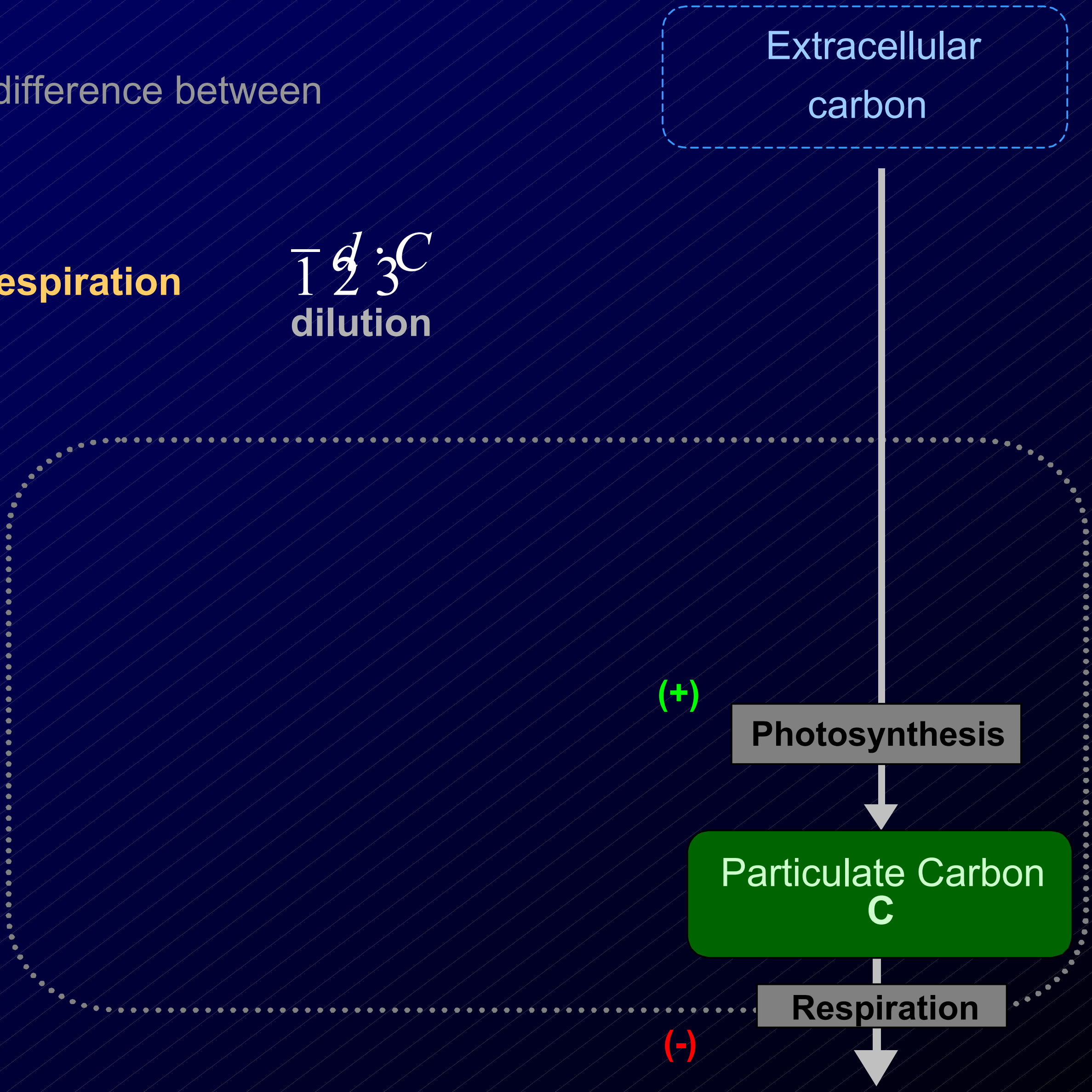
$$\frac{dC}{dt} = \textbf{Photosynthesis} - \textbf{Respiration} \quad - d \cdot C$$

dilution

- A part of the carbon is exported out of the chemostat.



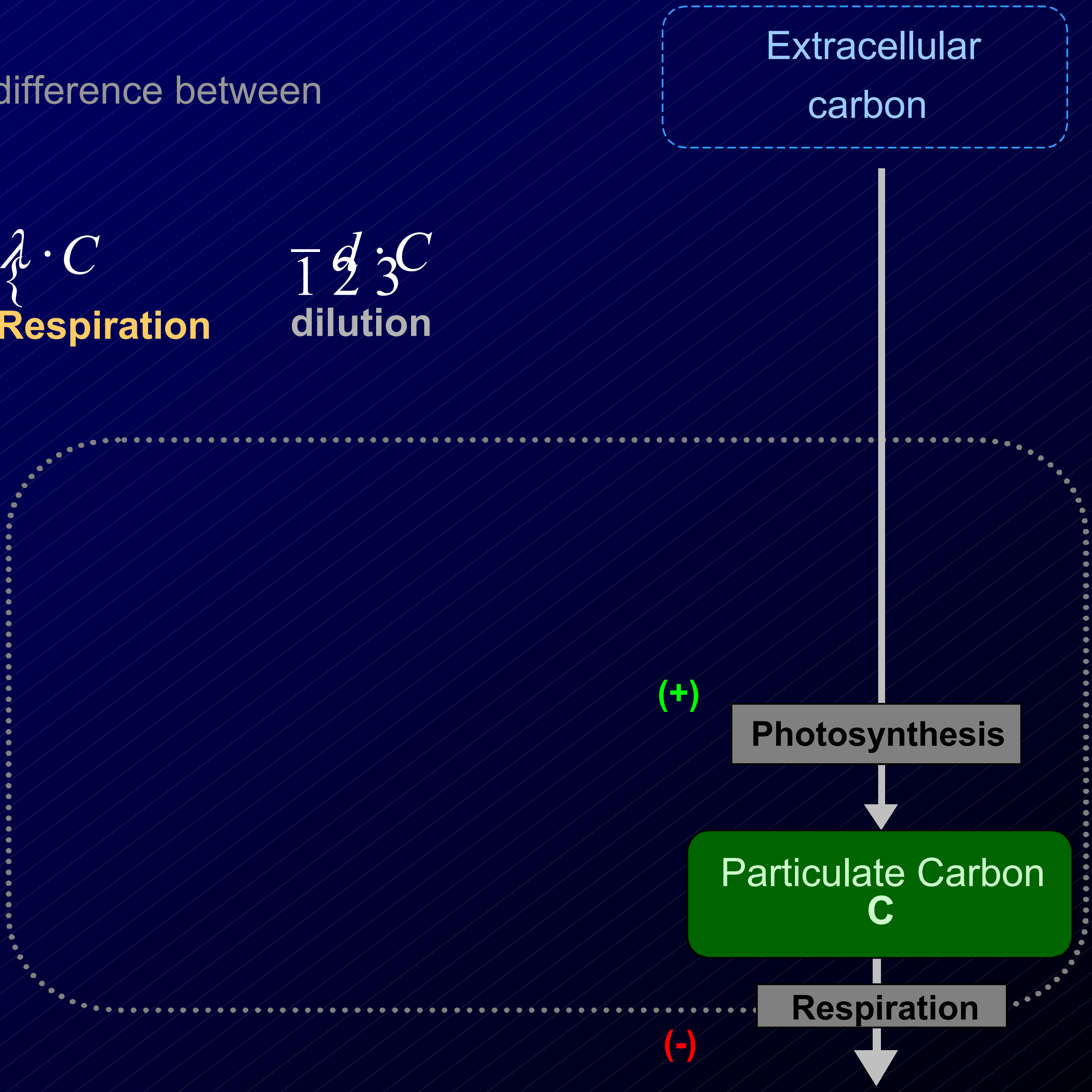
Hypotheses and formulations : Carbon

-Carbon variation is the result of the difference between photosynthesis and respiration.

$$\frac{dC}{dt} = \textbf{Photosynthesis} - \underbrace{\lambda \cdot C}_{\textbf{Respiration}} \underbrace{- d \cdot C}_{\textbf{dilution}}$$

- A part of the carbon is exported out of the chemostat.

- Respiration rate λ is constant.



Extracellular carbon

(+)

Photosynthesis

Particulate Carbon
C

Respiration

(-)

Hypotheses and formulations : Carbon

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$$\frac{dC}{dt} = \underbrace{a' \cdot L}_{\text{Photosynthesis}} - \underbrace{\lambda \cdot C}_{\text{Respiration}} - \underbrace{d \cdot C}_{\text{dilution}}$$

- A part of the carbon is exported out of the chemostat.

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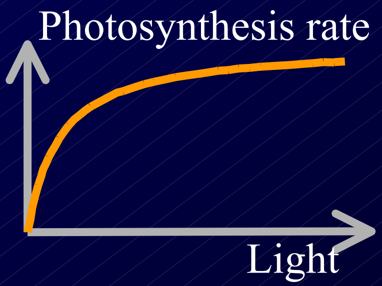
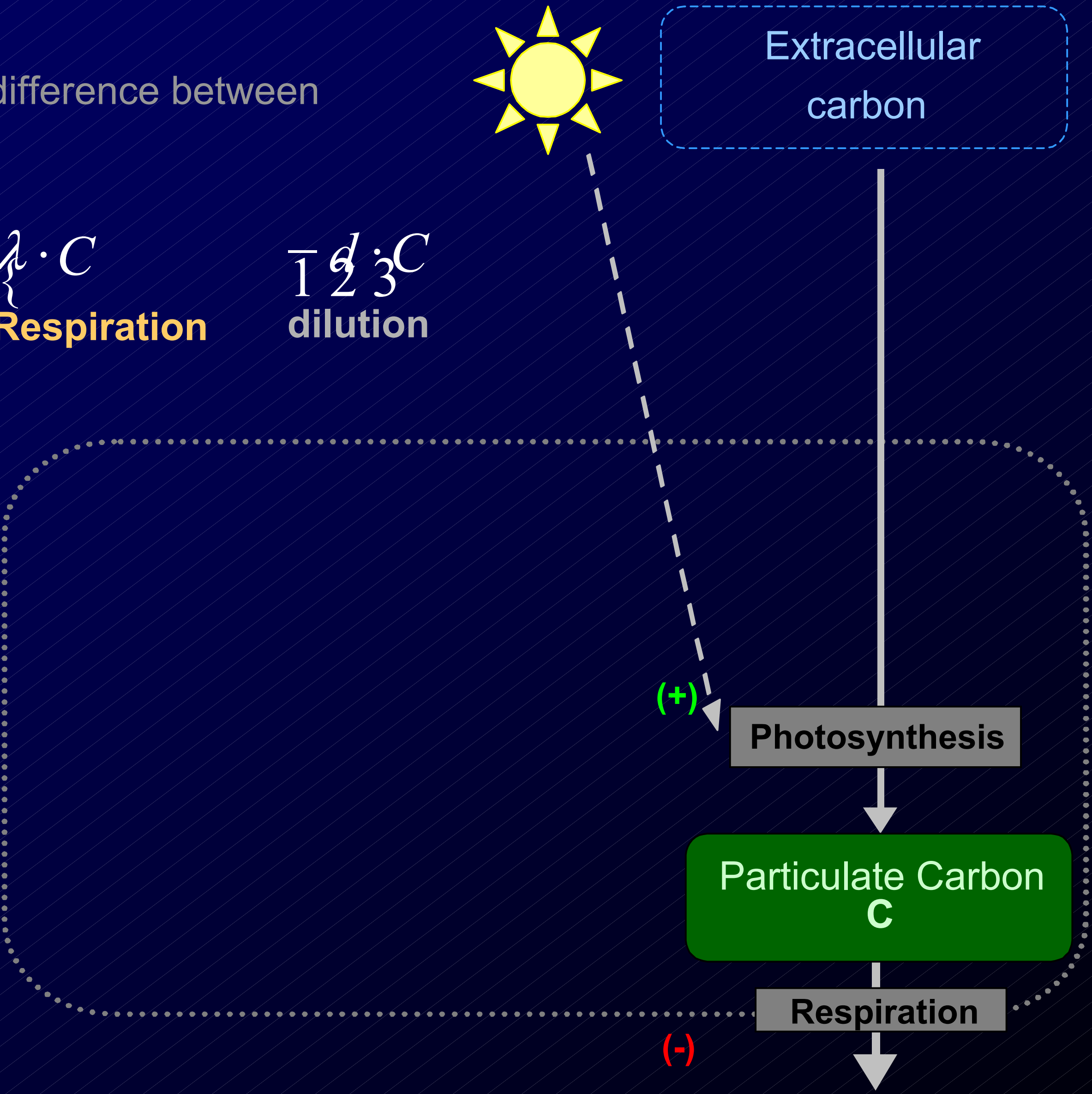
- Photosynthesis depends on:
  - light intensity (a '=f(i))

$$a' = \frac{\alpha \cdot i}{i + ki}$$





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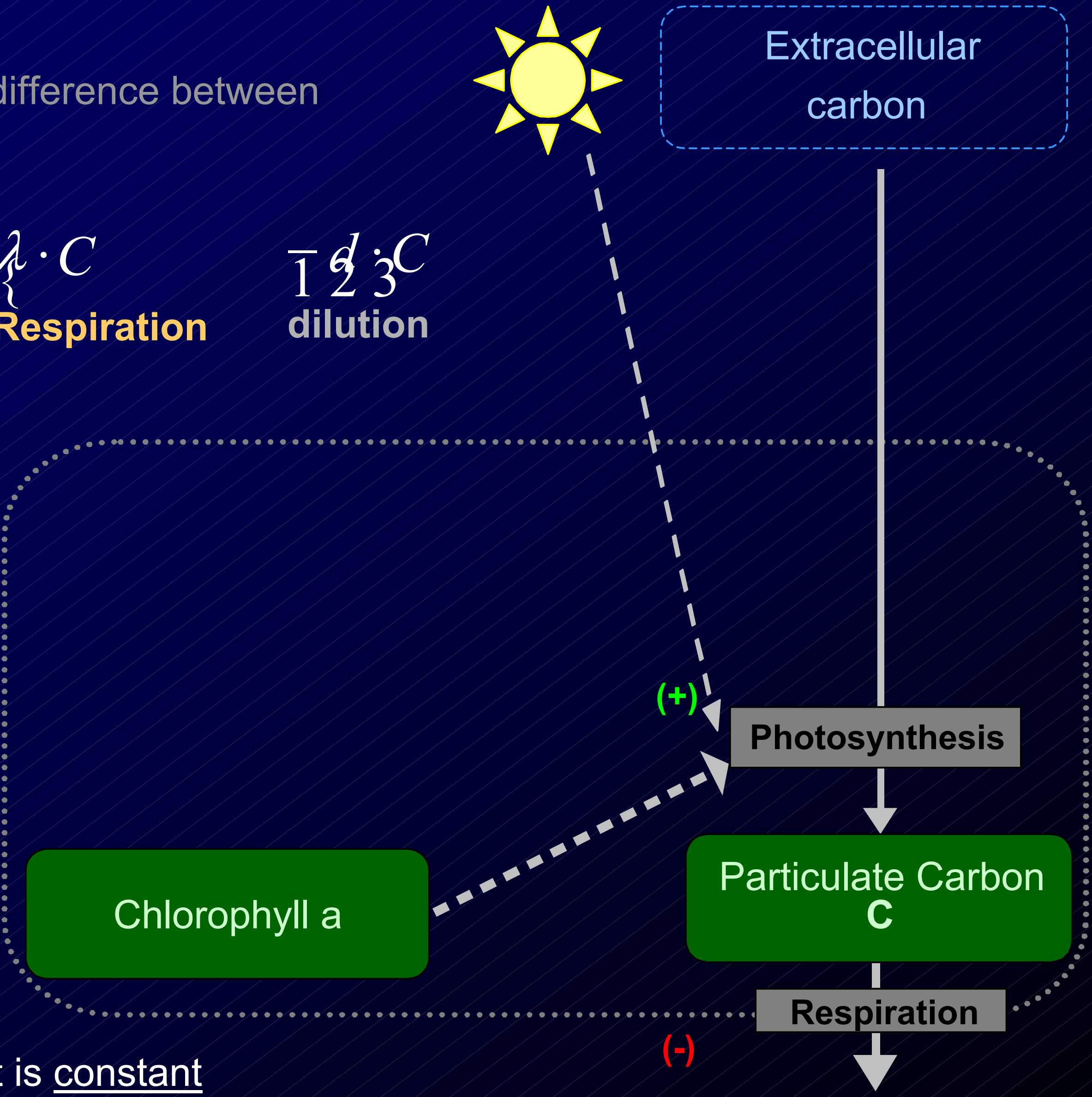
- A part of the biomass is exported out of the chemostat.

- Respiration rate λ is constant.

- Photosynthesis depends on:
  - light intensity (a ’=f(i))
  - chlorophyll a (L)

-Quantum yield is <u>constant</u>

-Chl a Specific absorption coefficient is <u>constant</u>



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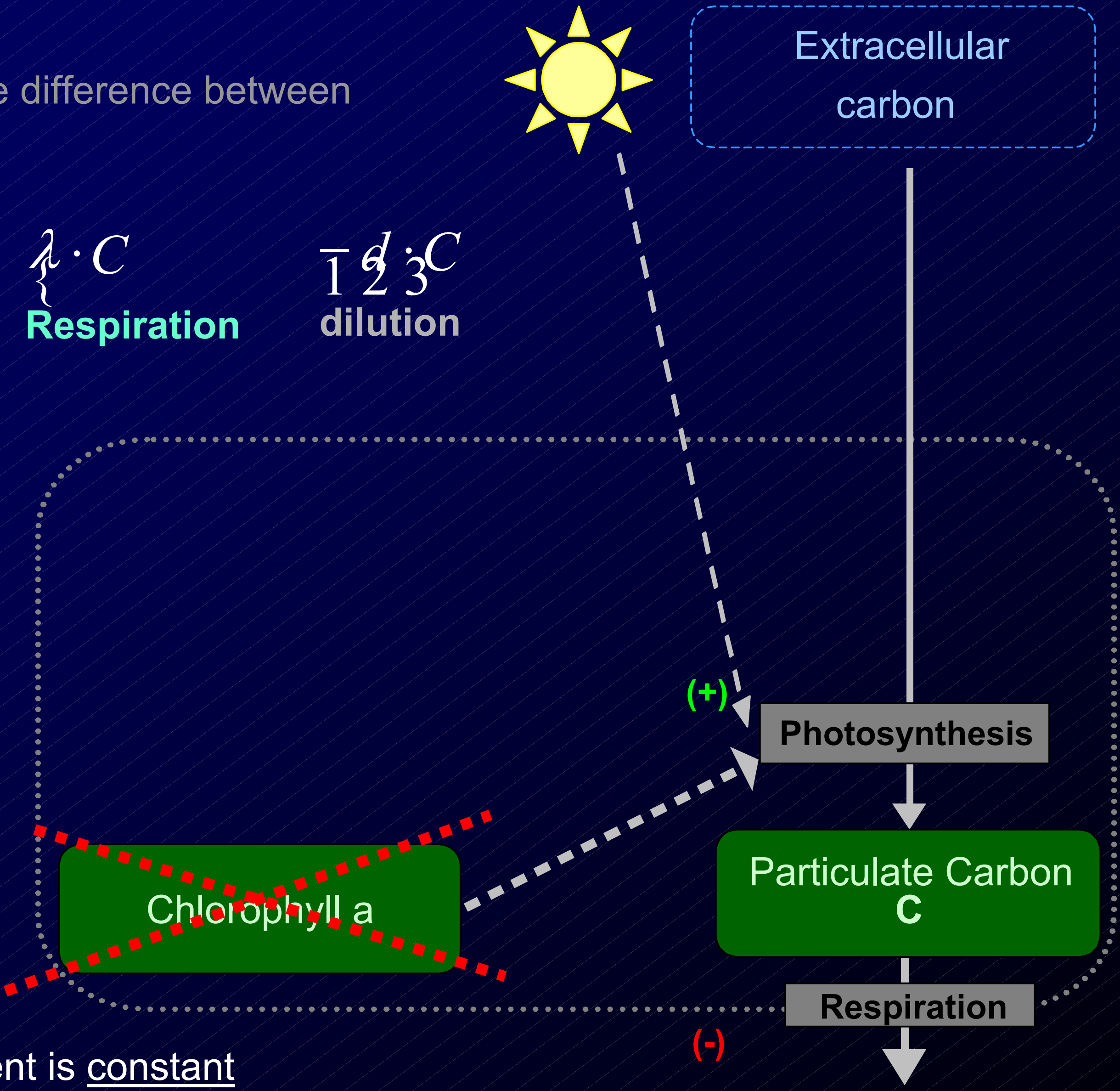

Extracellular carbon

(+)

Photosynthesis

~~Chlorophyll a~~

Particulate Carbon
C

Respiration

(-)

- Chlorophyll is represented as particulate chlorophyllian nitrogen concentration !

Chlorophyll and particulate nitrogen

- Chlorophyll is expressed in particulate chlorophyllian nitrogen concentrations !

- Total Particulate Nitrogen is divided in 2 pools:

Total
Particulate
Nitrogen

Nt = L+N

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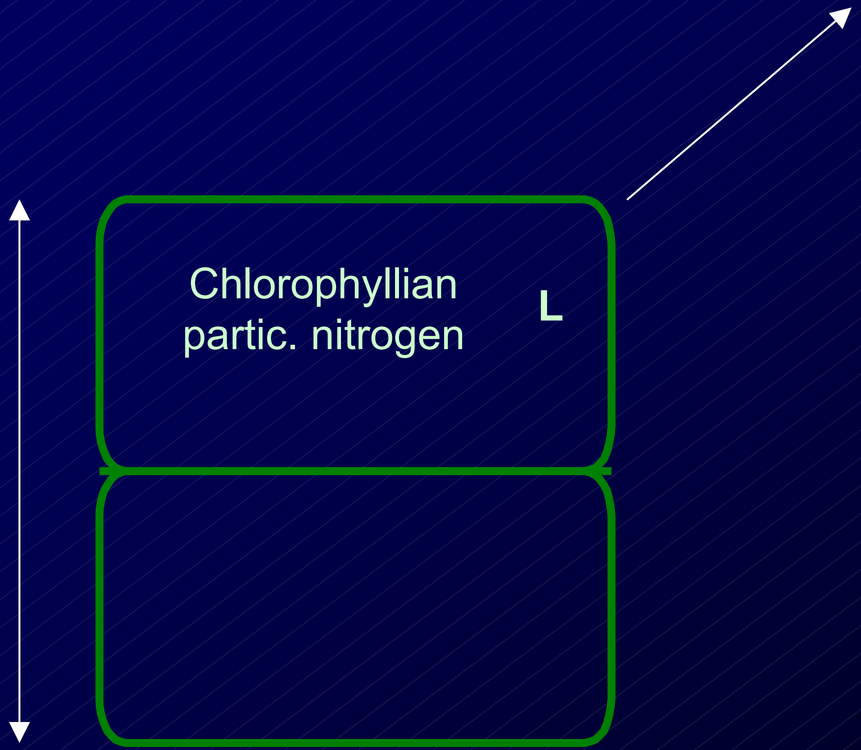

Nitrogen allocated to the
molecular structures
of Chlorophyll *a*

Chlorophyllian
partic. nitrogen

L

Total
Particulate
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Nt = L+N

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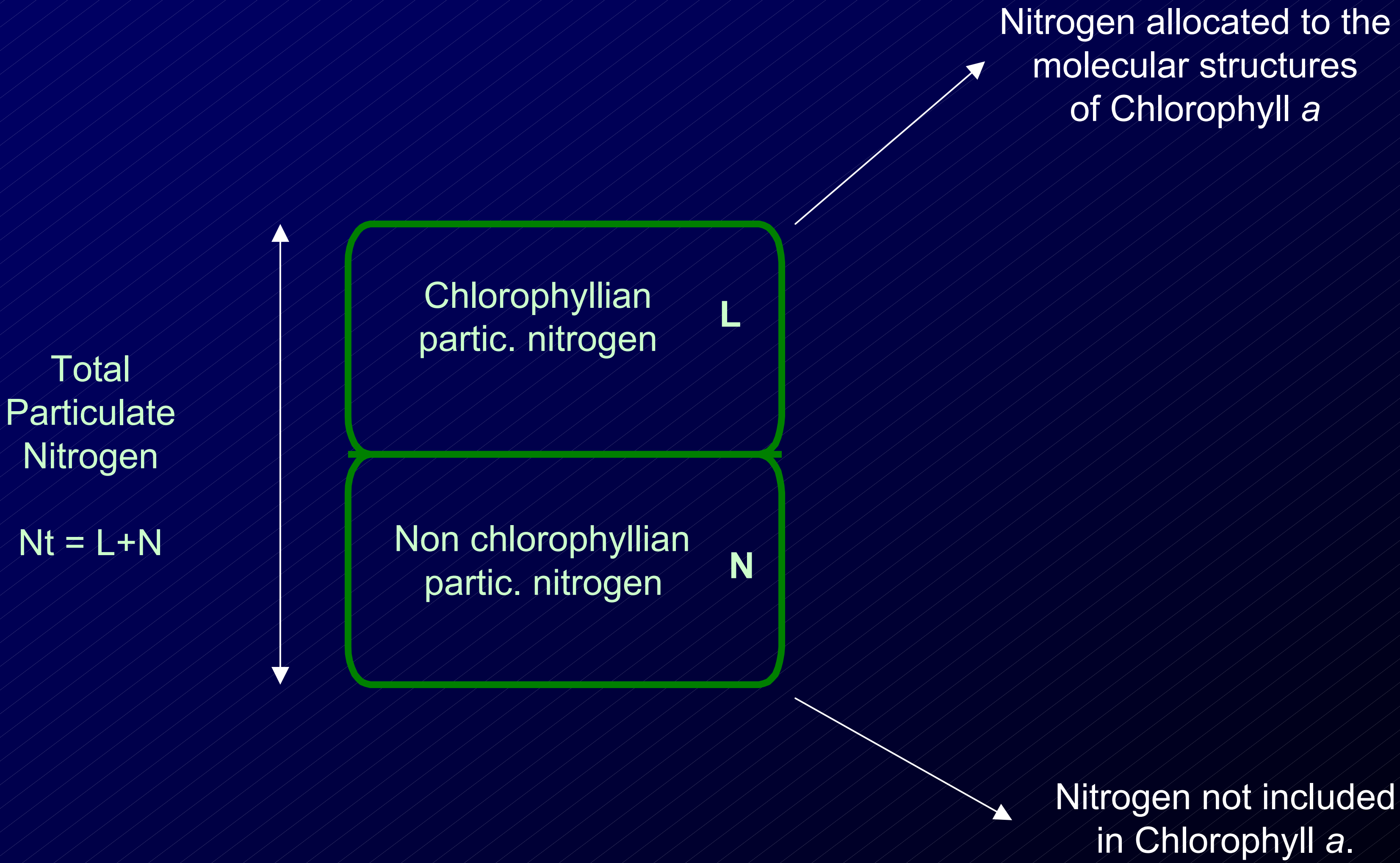

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Total
Particulate
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Chlorophyllian
partic. nitrogen **L**

Non chlorophyllian
partic. nitrogen **N**

Nitrogen not included
in Chlorophyll *a*.

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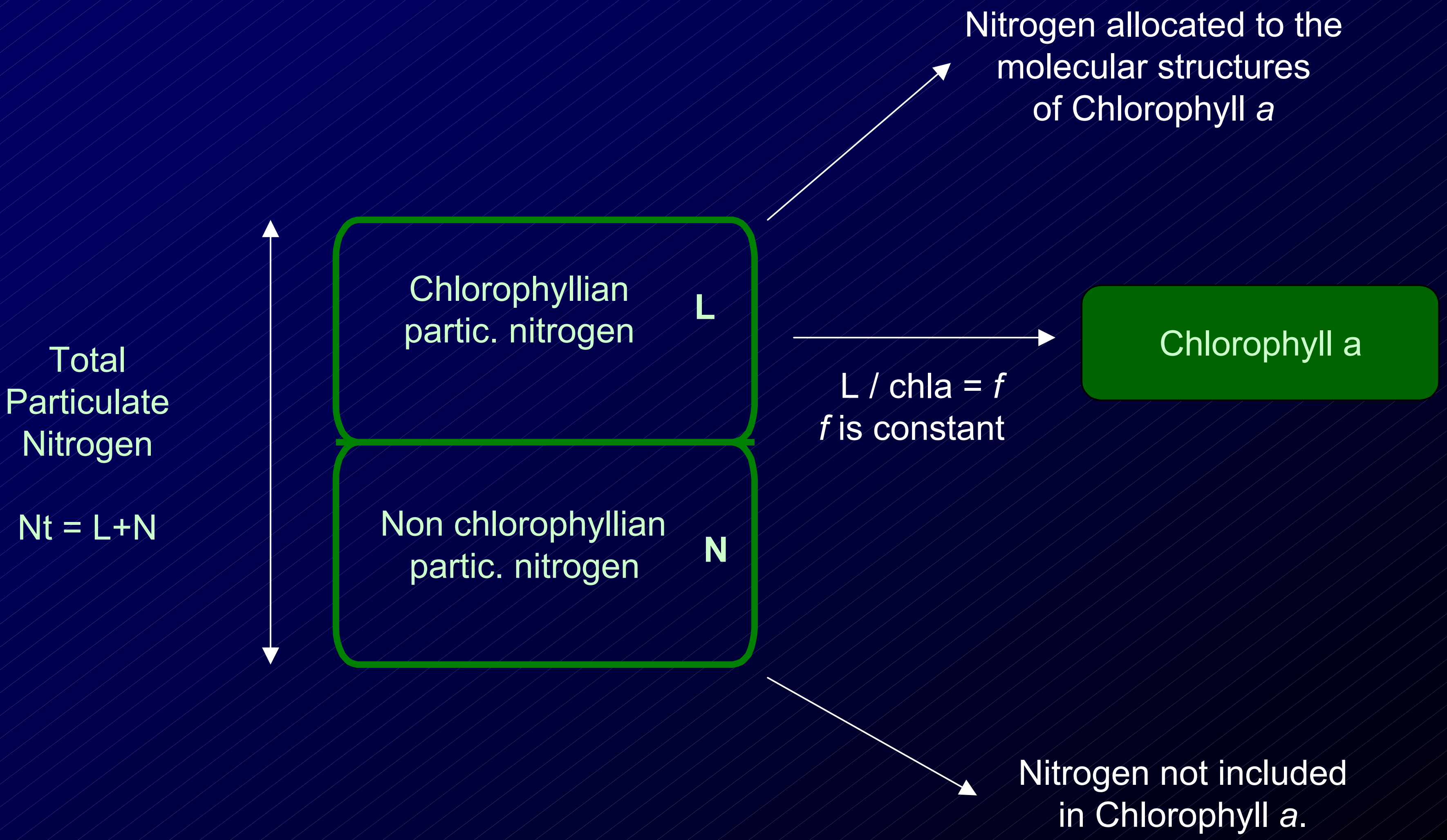

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Chlorophyllian
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Non chlorophyllian
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L / chla = f
f is constant

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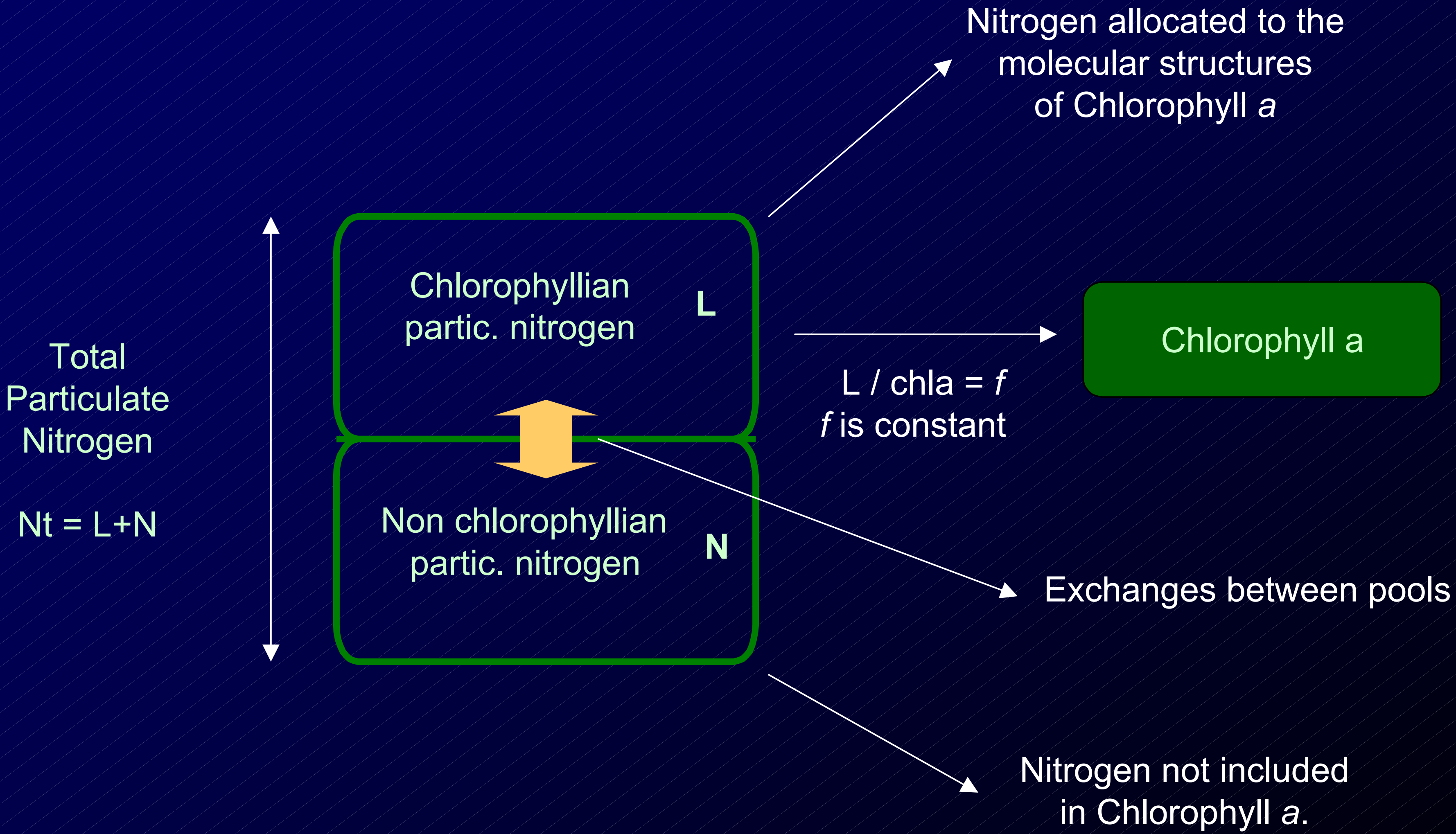

Nitrogen allocated to the
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Total
Particulate
Nitrogen

$Nt = L+N$

Chlorophyllian
partic. nitrogen **L**

Non chlorophyllian
partic. nitrogen **N**

Chlorophyll a

$L / chla = f$
f is constant

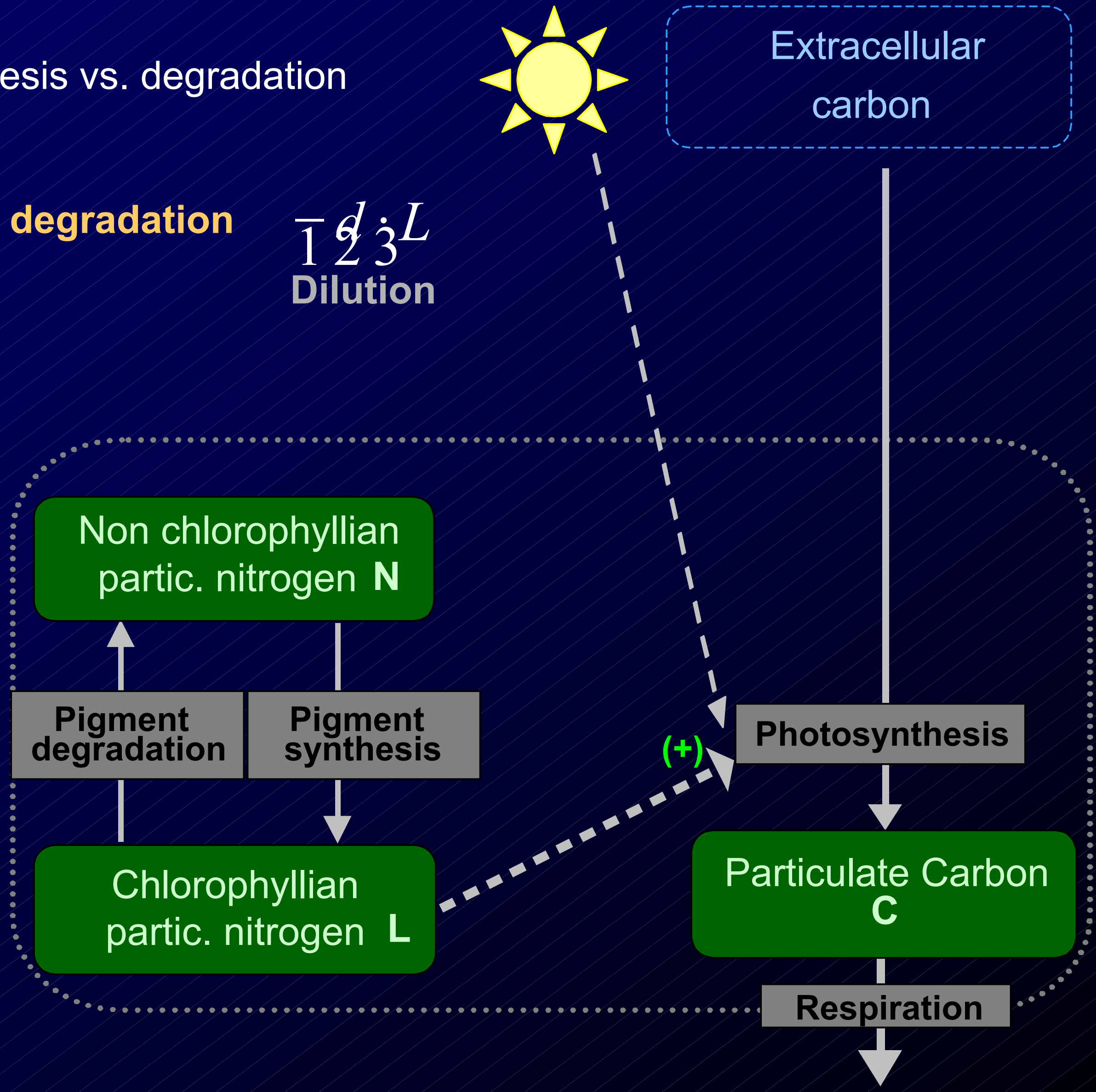
Exchanges between pools

Nitrogen not included
in Chlorophyll *a*.

Hypotheses and formulations : Pigments

- Chlorophyllian nitrogen pool : synthesis vs. degradation

$$\frac{dL}{dt} = \text{Pigment synthesis} - \text{degradation} \underbrace{-d \cdot L}_{\text{Dilution}}$$



Extracellular carbon

Non chlorophyllian partic. nitrogen **N**

Pigment degradation

Pigment synthesis

Chlorophyllian partic. nitrogen **L**

(+)

Photosynthesis

Particulate Carbon **C**

Respiration

Hypotheses and formulations : Pigments

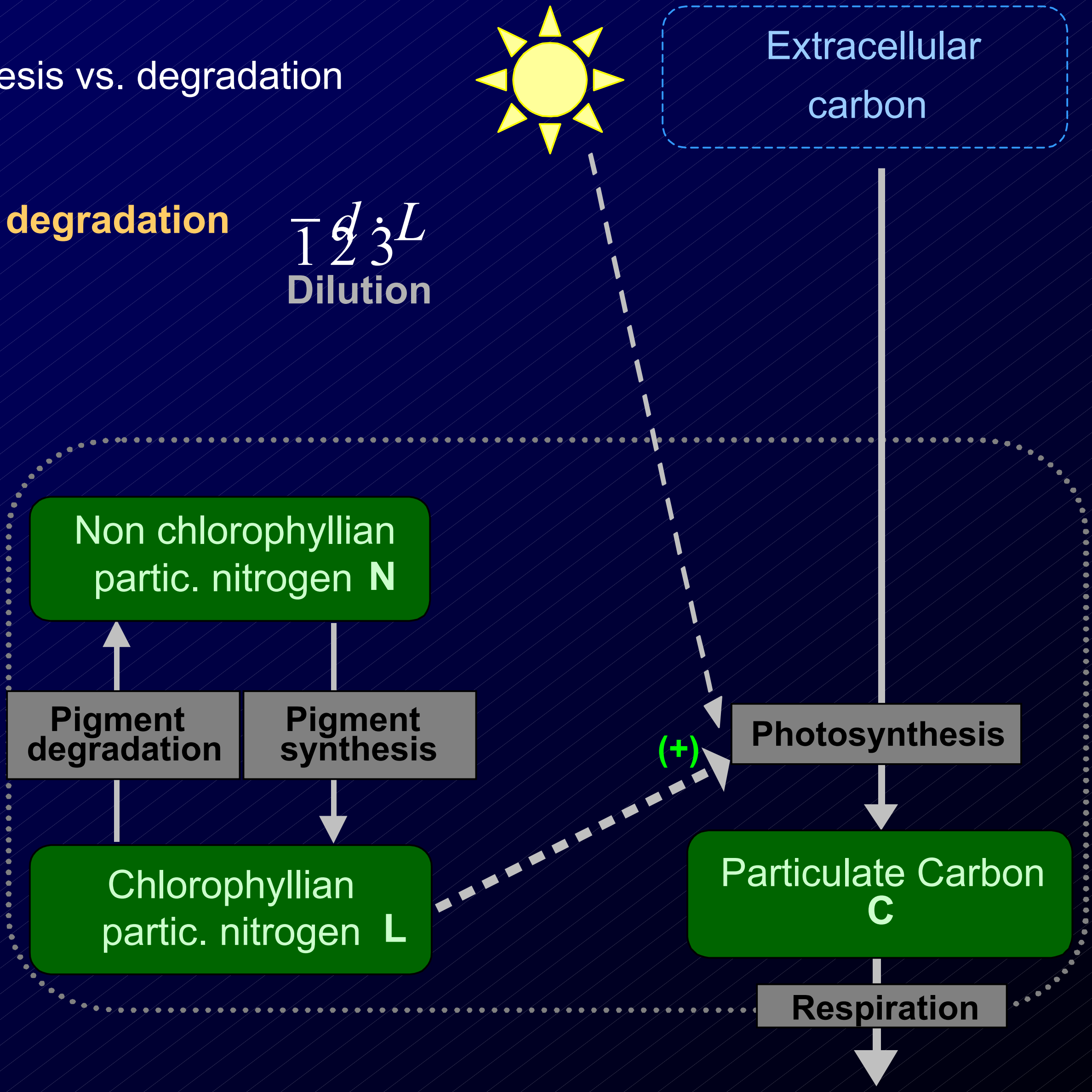
- Chlorophyllian nitrogen pool : synthesis vs. degradation

$$\frac{dL}{dt} = \underbrace{k' \cdot N \cdot a' \frac{L}{C}}_{\text{Pigment synthesis}} - \text{degradation} - \underbrace{d \cdot L}_{\text{Dilution}}$$

-Synthesis term is designed to integrate…

→ *Photoacclimation*

→ *Compensation phenomenon*



Regulation of pigment synthesis

Synthesis depends on…

Chlorophyllian nitrogen synthesis rate $= \boxed{N} \cdot \boxed{k'} \cdot \boxed{a' \cdot \frac{L}{C}}$

Non chlorophyllian nitrogen pool

(+)

Growth rate

(+)

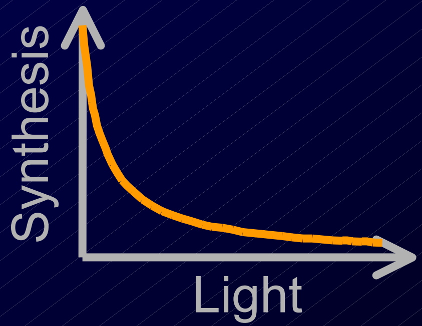
Light intensity

(+)

Output from the model:

$$\mu_{GROSS} = \frac{1}{C} \cdot \frac{dC}{dt} + \lambda = a' \frac{L}{C}$$

$$k' = \frac{kl \cdot kc}{i + kc}$$



Hypotheses and formulations : Pigments

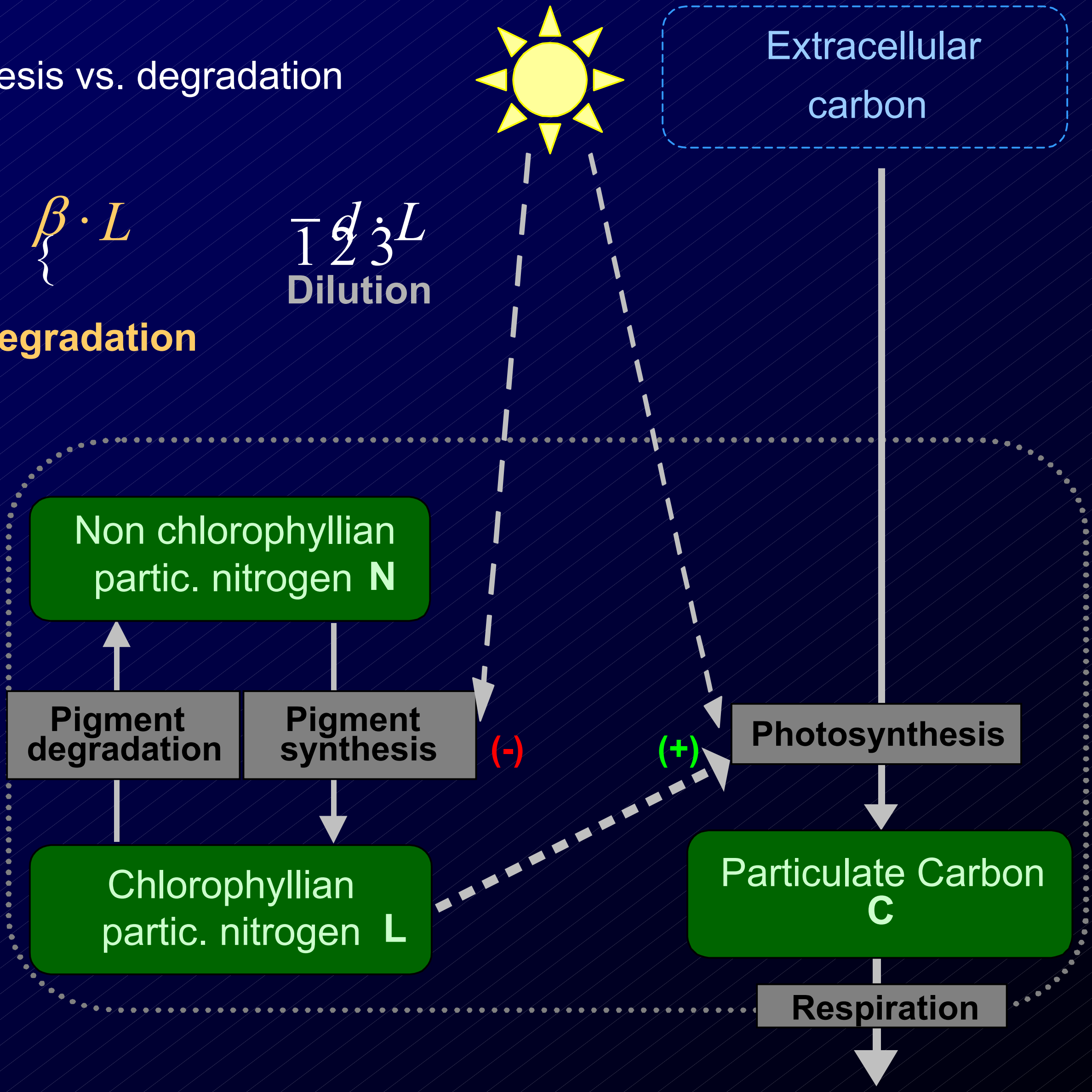
- Chlorophyllian nitrogen pool : synthesis vs. degradation

$$\frac{dL}{dt} = \underbrace{k'\cdot N\cdot a'\frac{L}{C}}_{\text{Pigment synthesis}} - \underbrace{\beta\cdot L}_{\text{degradation}} - \underbrace{d\cdot L}_{\text{Dilution}}$$

-Synthesis depends on:

- - non chlor. Nitrogen (+)
  - light (-)
  - growth rate (+)

-Degradation rate β is constant.



Extracellular carbon

Non chlorophyllian partic. nitrogen **N**

Pigment degradation

Pigment synthesis

(-)

(+)

Photosynthesis

Chlorophyllian partic. nitrogen **L**

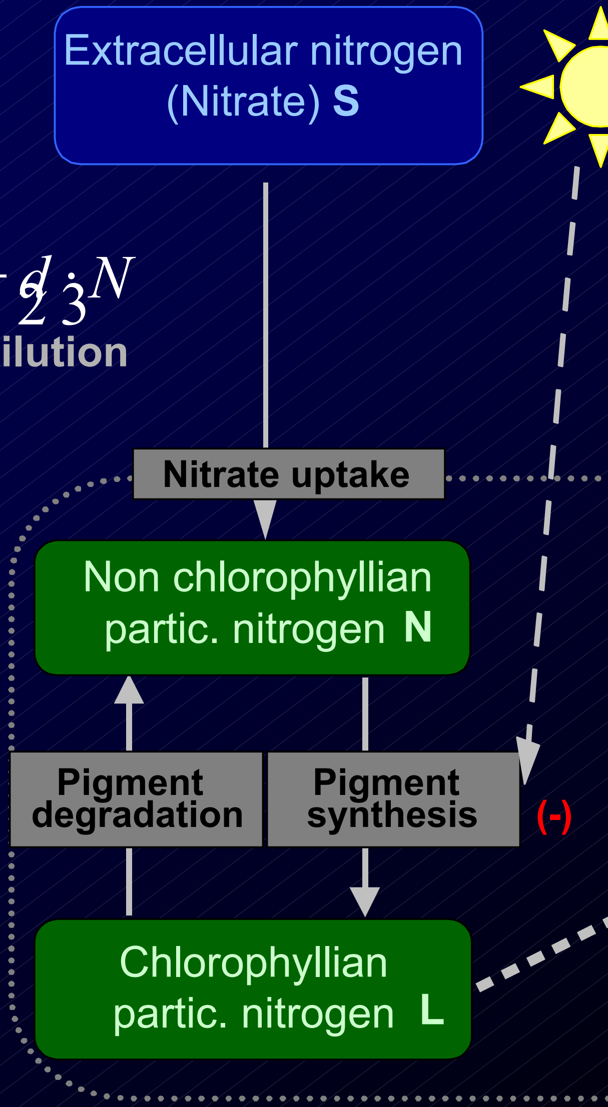
Particulate Carbon **C**

Respiration

Hypotheses and formulations : Non Chlorophyllian Nitrogen Pool

Non Chlorophyllian nitrogen pool:

$$\frac{dN}{dt} = -\underbrace{k' \cdot N \cdot a' \frac{L}{C}}_{\text{Pigment synthesis}} + \underbrace{\beta \cdot L}_{\text{degradation}} + \underbrace{\rho m \cdot \frac{S}{S+ks} \cdot C}_{\text{Nitrate uptake}} - \underbrace{d \cdot N}_{\text{Dilution}}$$



- Gain from pigment degradation

- Losses from pigment synthesis and from dilution

- Gain from Nitrate uptake

- Uptake by the cell depends only on the extracellular nitrate concentration

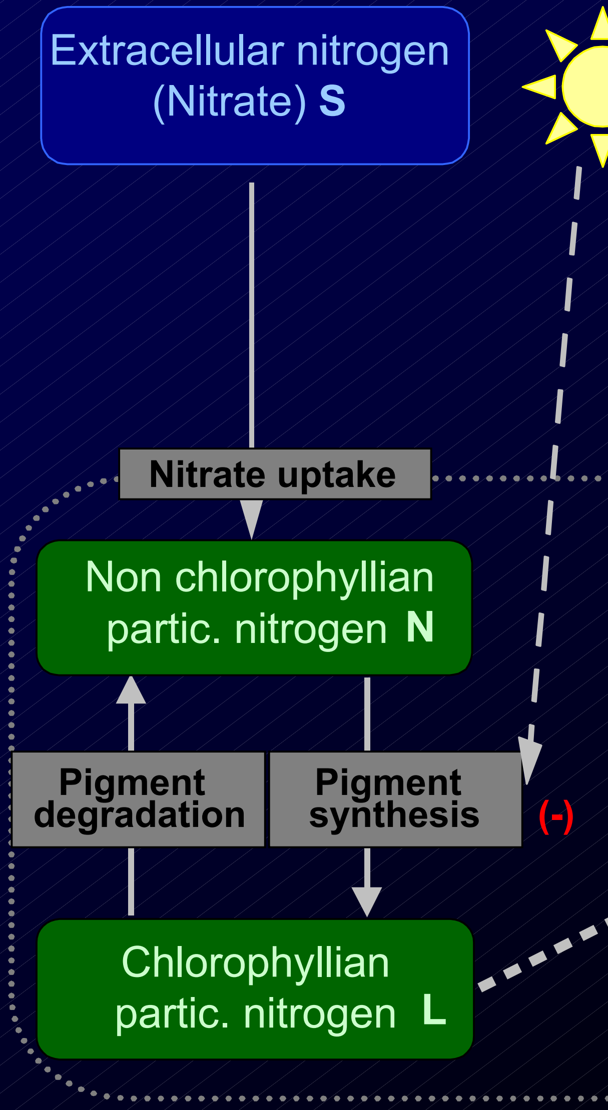
Hypotheses and formulations : Nitrate

$$\frac{dS}{dt} = \underbrace{d \cdot (Sin - S)} - \underbrace{\rho m \cdot \frac{S}{S+ks} \cdot C}$$

Nitrate input - Dilution **Nitrate uptake**

-Input of nitrate at concentration *Sin* by renewal of culture medium at dilution *d*.

- Uptake by the cell



Extracellular nitrogen (Nitrate) **S**

Nitrate uptake

Non chlorophyllian partic. nitrogen **N**

Pigment degradation

Pigment synthesis

(-)

Chlorophyllian partic. nitrogen **L**

Equations

Nitrate

$$\frac{dS}{dt} = \underbrace{d \cdot (Sin - S)}_{\text{Input - Dilution}} - \underbrace{\rho m \cdot \frac{S}{S + ks} \cdot C}_{\text{uptake}}$$

Non chlorophyllian particulate nitrogen

$$\frac{dN}{dt} = \underbrace{-d \cdot N}_{\text{Dilution}} + \underbrace{\rho m \cdot \frac{S}{S + ks} \cdot C}_{\text{uptake}} - \underbrace{k' N \cdot a' \frac{L}{C}}_{\text{chlorophyll synthesis}} + \underbrace{\beta \cdot L}_{\text{pigment degradation}}$$

Chlorophyllian nitrogen

$$\frac{dL}{dt} = \underbrace{-d \cdot L}_{\text{Dilution}} + \underbrace{k' N \cdot a' \frac{L}{C}}_{\text{chlorophyll synthesis}} - \underbrace{\beta \cdot L}_{\text{pigment degradation}}$$

particulate carbon

$$\frac{dC}{dt} = \underbrace{-d \cdot C}_{\text{Dilution}} + \boxed{\underbrace{a' \cdot L}_{\text{Photosynthesis}} - \underbrace{\lambda \cdot C}_{\text{Respiration}}} \rightarrow$$

Net carbon fixation flux

Interesting caracteristics of BioLOV

- Phytoplankton growth models often use 2 types of parameters that BioLOV does not use: *Growth rate , quotas (minimal, maximal)*

- These parameters are outputs from BioLOV equations.

  - Growth rate

$$\mu_{net} = \frac{1}{C} \cdot \frac{dC}{dt} = a'\frac{L}{C} - \lambda$$

  - Chlorophyll:carbon ratio

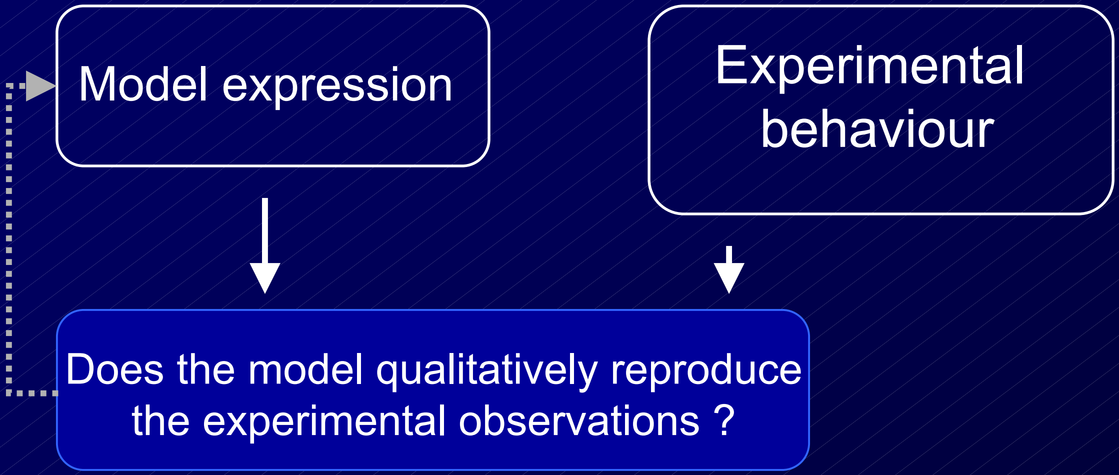
$$\frac{Chla}{C} = \frac{1}{f} \cdot \frac{L}{C}$$

  - Nitrogen:carbon ratio

$$\frac{Nt}{C} = \frac{N+L}{C}$$

Qualitative properties

Modelling approach



Model expression

Experimental behaviour

Does the model qualitatively reproduce the experimental observations ?

→In this step, we test if mathematical properties evolve in the same way than observations for a change of light or dilution

→If a failure to do is observed, the model needs to be modified.

→Approach is purely based on formal calculus. This step does not take account of parameters values !

Steady-state solutions

Nitrate

$$S^* = \frac{ks \cdot d \cdot \left[k' \cdot (d+\lambda) + (d+\beta)\right]}{\rho m \cdot a' \cdot k' - d \cdot \left[k' \cdot (d+\lambda) + (d+\beta)\right]}$$

Non chlorophyllian particulate nitrogen

$$N^* = \frac{(d+\beta) \cdot (Sin - S^*)}{k' \cdot (d+\lambda) + (d+\beta)}$$

Chlorophyllian nitrogen

$$L^* = \frac{k' \cdot (d+\lambda) \cdot (Sin - S^*)}{k' \cdot (d+\lambda) + (d+\beta)}$$

Particulate carbon

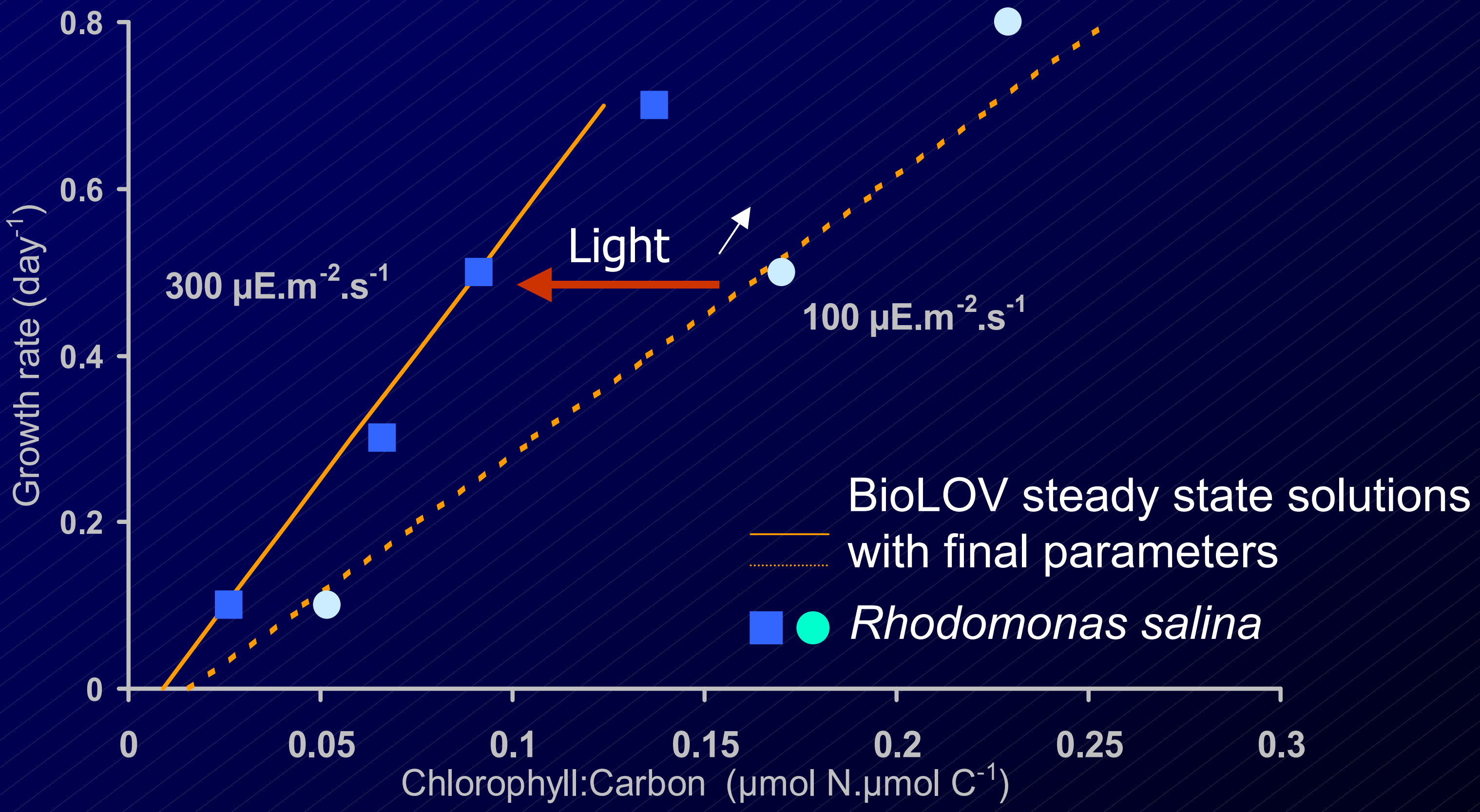
$$C^* = \frac{a' \cdot k' \cdot (Sin - S^*)}{k' \cdot (d+\lambda) + (d+\beta)}$$

$$\frac{N^*}{C^*} = \frac{(d+\beta)}{a' \cdot k'}$$

$$\frac{L^*}{C^*} = \frac{(d+\lambda)}{a'}$$

- Available measurements: chlorophyll (L*), Carbon (C*) , total particulate nitrogen (N+L)*

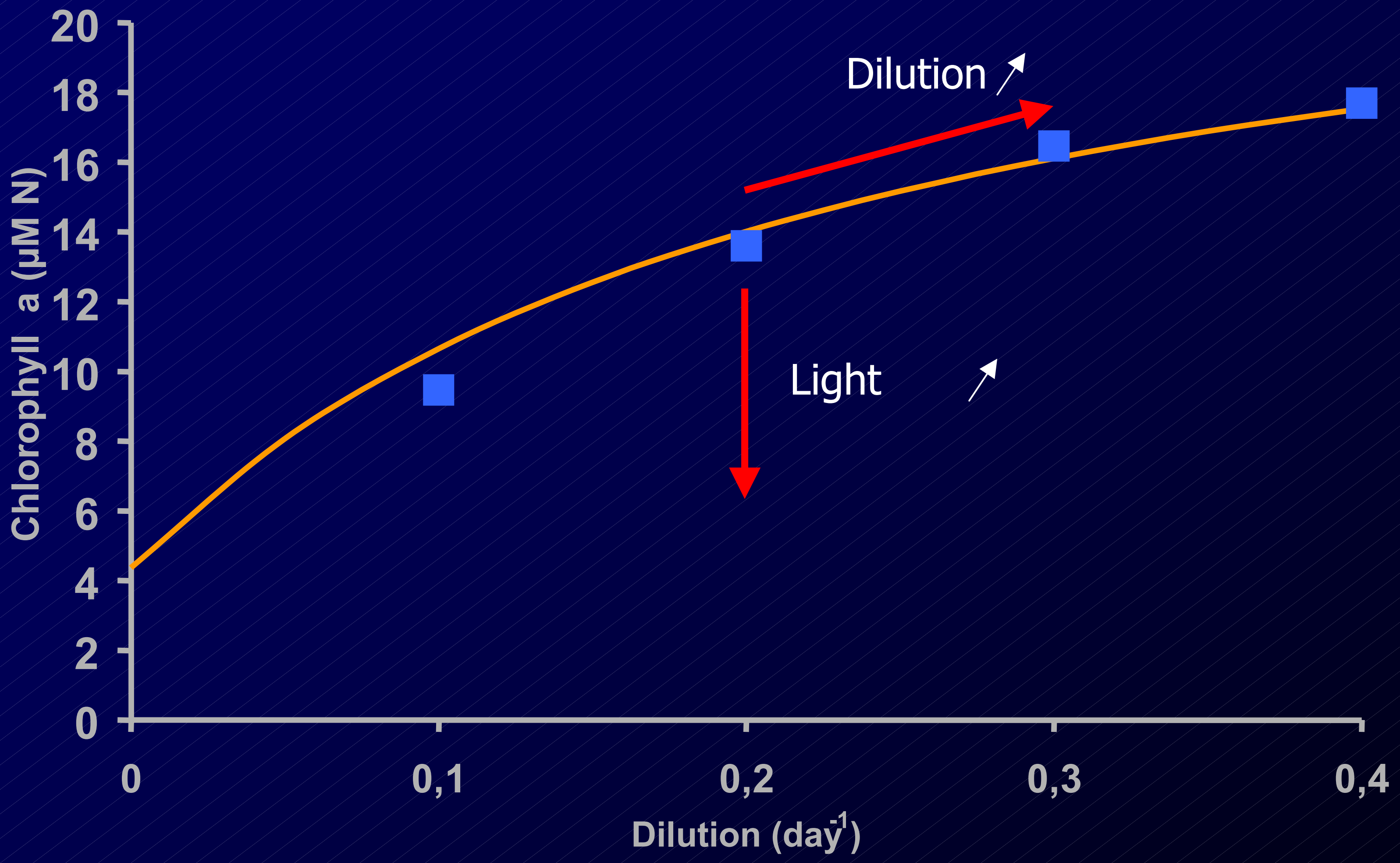
Observations vs. Model: Chlorophyll:Carbone (L:C) ratio



$$\frac{L^*}{C^*} = \frac{(d+\lambda)(i+k_i)}{\alpha i}$$

- Increases with dilution
- Decreases with light

Observations vs. Model: Chlorophyll

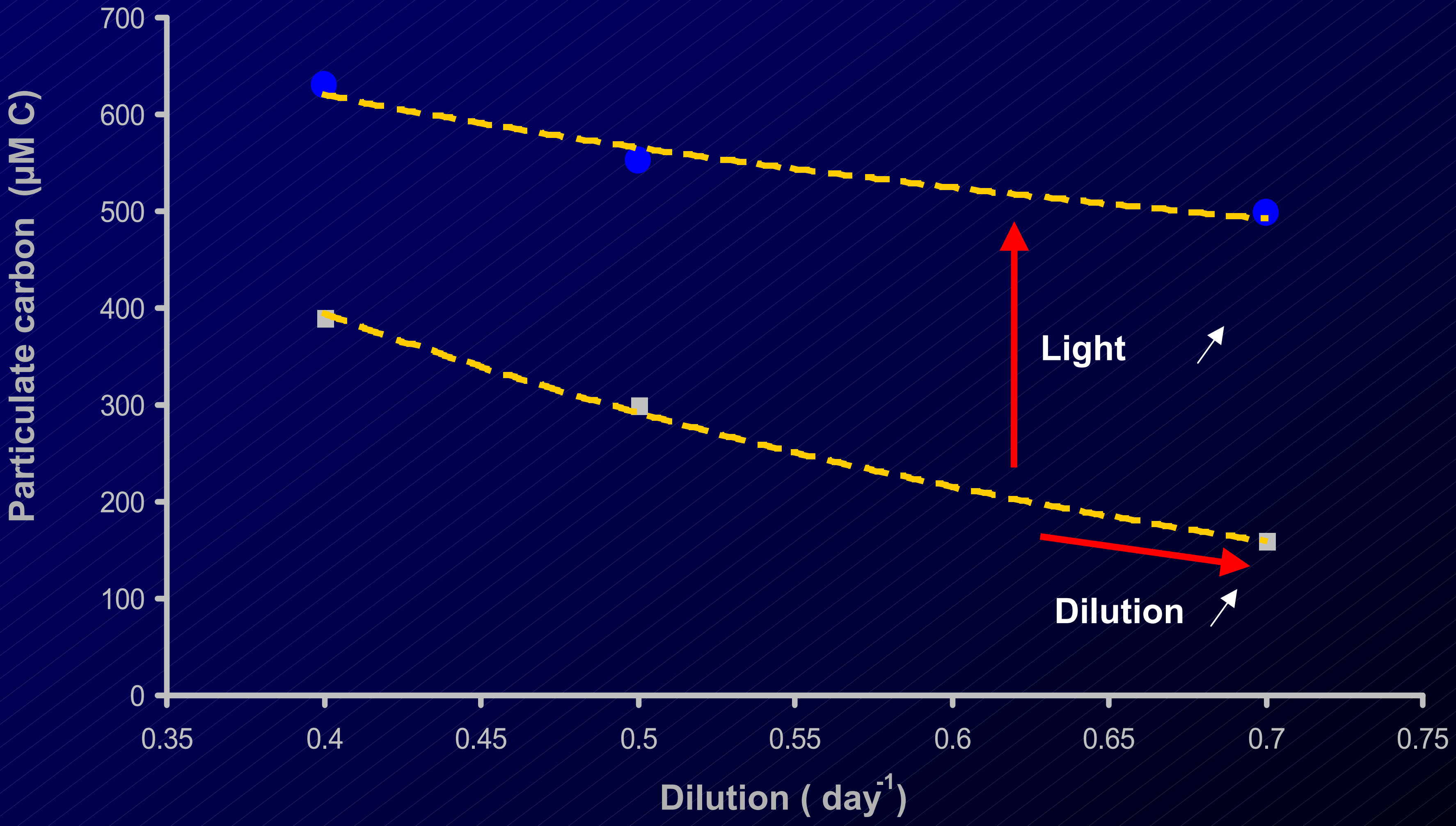


$$L^* = \frac{kckl \cdot (d + \lambda) \cdot Sin}{kckl \cdot (d + \lambda) + (d + \beta)(i + kc)}$$

- Increases with dilution

- decreases with light

Observation vs. Model: Particulate carbon



$$C^* = \frac{a' \cdot k' \cdot (Sin - S^*)}{k' \cdot (d + \lambda) + (d + \beta)}$$

- decreases with dilution

- increases with light

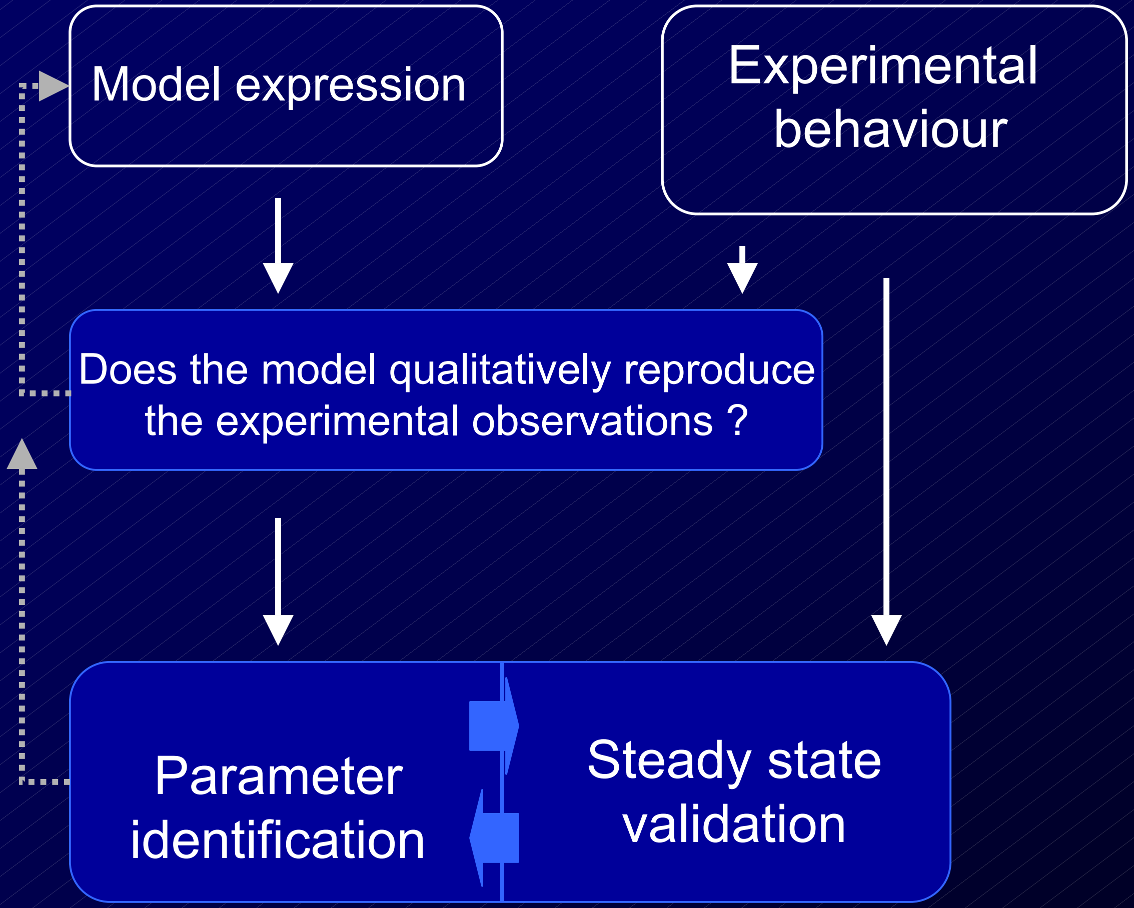
Summary of qualitative properties

	Increase of	
Variable	**Light intensity**	**Dilution rate**
$C^{\dagger}$	↗	↘
$L^{\dagger}$	↘	↗
$N^{\dagger}$	↗	↘
$N^{\dagger} / C^{\dagger}$	↘	↗
$L^{\dagger} / C^{\dagger}$	↘	↗

→ Model behaviour is coherent with observations.

Parameter identification

Modelling approach



Model expression

Experimental behaviour

Does the model qualitatively reproduce the experimental observations ?

Parameter identification

Steady state validation

→ Development of mathematical methods that simultaneously estimate parameters from data and also validate again model structure

Parameter identification

Ex: $$\frac{Chla^*}{C^*}=\frac{(d+\lambda)(i+k_i)}{f\alpha i}=\frac{d}{f\alpha}+\frac{dk_i}{f\alpha i}+\frac{\lambda}{f\alpha}+\frac{\lambda k_i}{f\alpha i}$$

2 dilutions rate *d1, d2* and same intensity *I*:

$$\left.\frac{Chla}{C}\right|_{d2}=d2\cdot\left(\frac{1}{f\cdot\alpha}+\frac{ki}{f\cdot\alpha}\cdot\frac{1}{I}\right)+\frac{\lambda}{f\cdot\alpha}$$

$$\left.\frac{Chla}{C}\right|_{d1}=d1\cdot\left(\frac{1}{f\cdot\alpha}+\frac{ki}{f\cdot\alpha}\cdot\frac{1}{I}\right)+\frac{\lambda}{f\cdot\alpha}$$

d1-d2

$$\left.\frac{Chla}{C}\right|_{d1}-\left.\frac{Chla}{C}\right|_{d2}=(d1-d2)\cdot\left(\frac{1}{f\cdot\alpha}+\frac{ki}{f\cdot\alpha}\cdot\frac{1}{I}\right)$$

Parameter identification

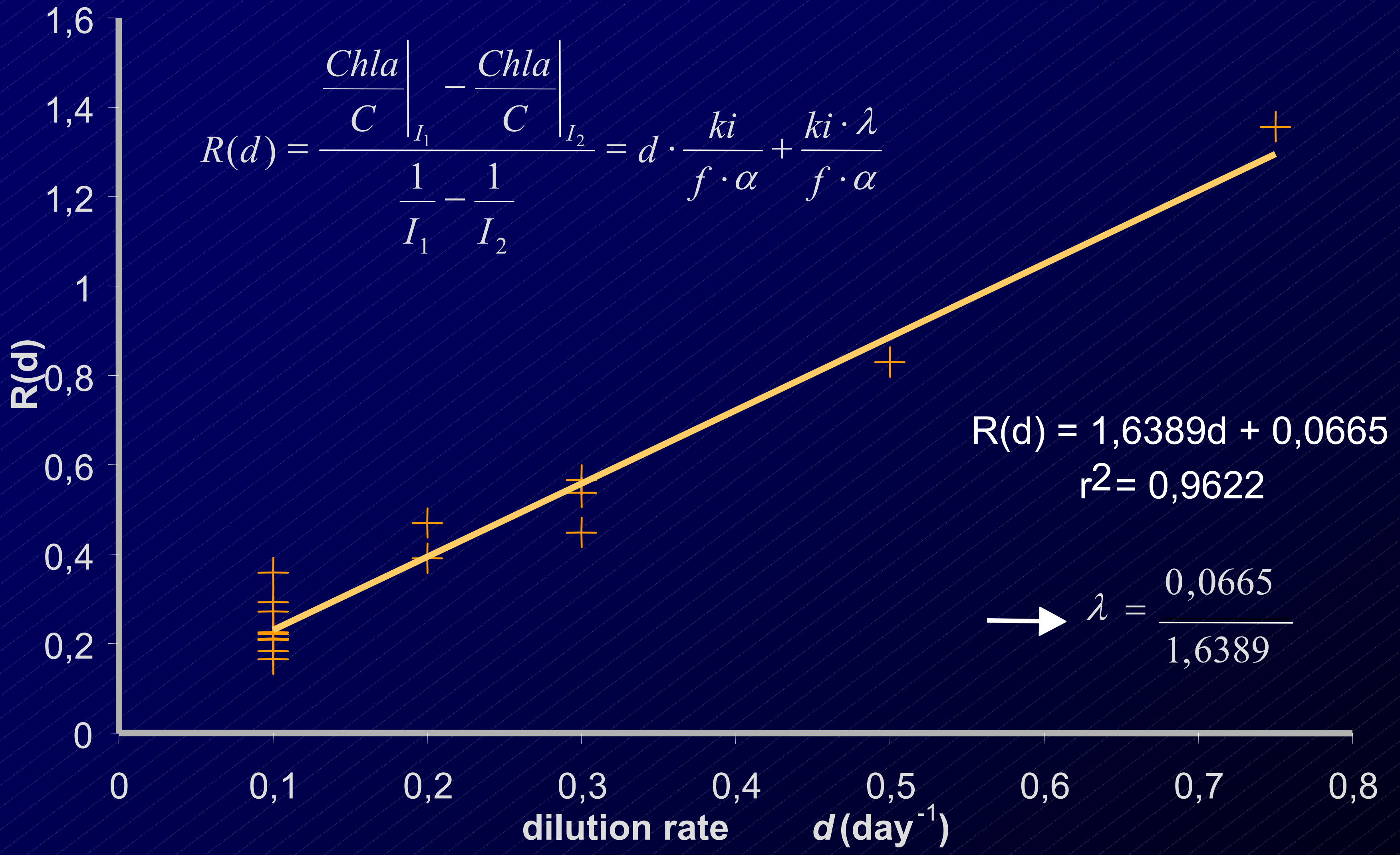
$$\left.\frac{Chla}{C}\right|_{d1}-\left.\frac{Chla}{C}\right|_{d2}=(d1-d2)\cdot\left(\frac{1}{f\cdot\alpha}+\frac{ki}{f\cdot\alpha}\cdot\frac{1}{I}\right)$$

$$\boxed{\frac{\left.\frac{Chla}{C}\right|_{d_1}-\left.\frac{Chla}{C}\right|_{d_2}}{d_1-d_2}}=\boxed{\frac{1}{I}}\cdot\underbrace{\frac{ki}{f\cdot\alpha}}_{A}+\underbrace{\frac{1}{f\cdot\alpha}}_{B}$$

→ Each term is known . A linear regression is applied on data

→ A/B gives *ki*

→ This method also works with 2 constant values of I, a variable dilution rate and for the following ratios: $\frac{\mathrm{Chla}}{\mathrm{C}},\frac{\mathrm{Nt}}{\mathrm{C}},\frac{\mathrm{Nt}}{\mathrm{Chla}}$



$$R(d) = \frac{\left.\frac{Chla}{C}\right|_{I_1} - \left.\frac{Chla}{C}\right|_{I_2}}{\frac{1}{I_1} - \frac{1}{I_2}} = d \cdot \frac{ki}{f \cdot \alpha} + \frac{ki \cdot \lambda}{f \cdot \alpha}$$

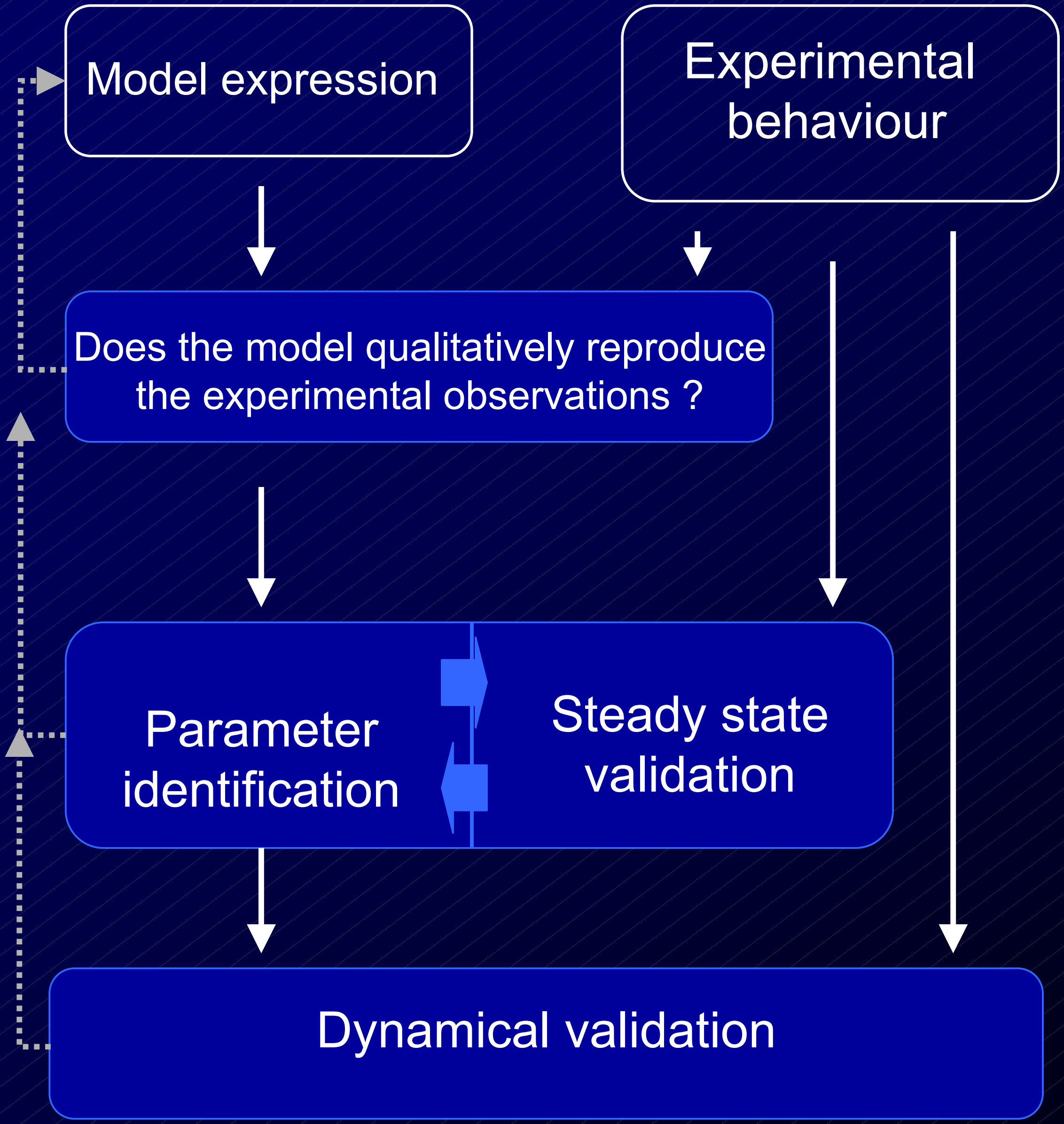
R(d) = 1,6389d + 0,0665
$r^2 = 0,9622$

$$\rightarrow \lambda = \frac{0,0665}{1,6389}$$

- → Allows the determination of all parameters (except *ρm* et *ks*).
- → very simple : linear regressions...

Model vs. Data

Modelling approach



Model expression

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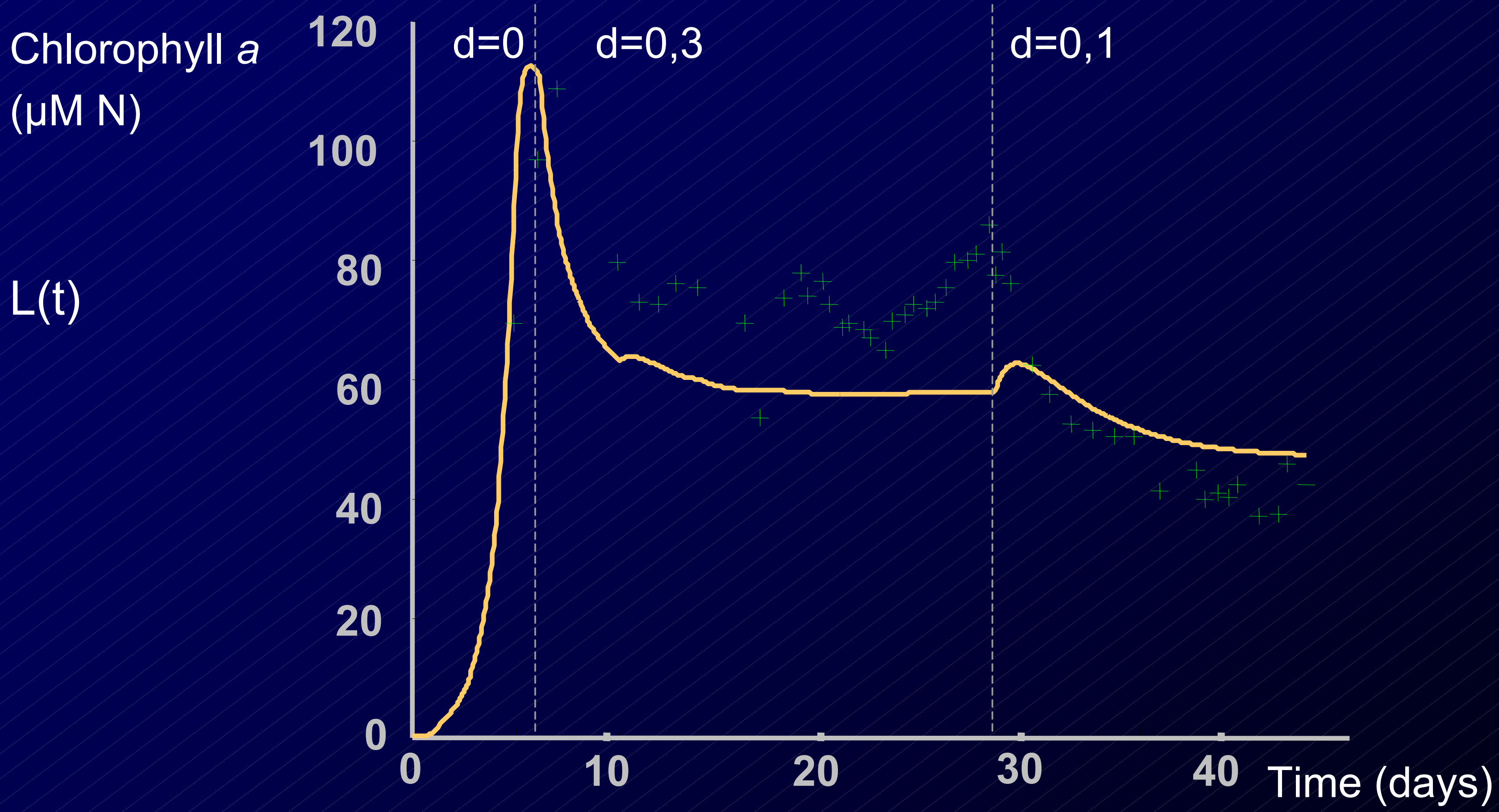
Parameter identification

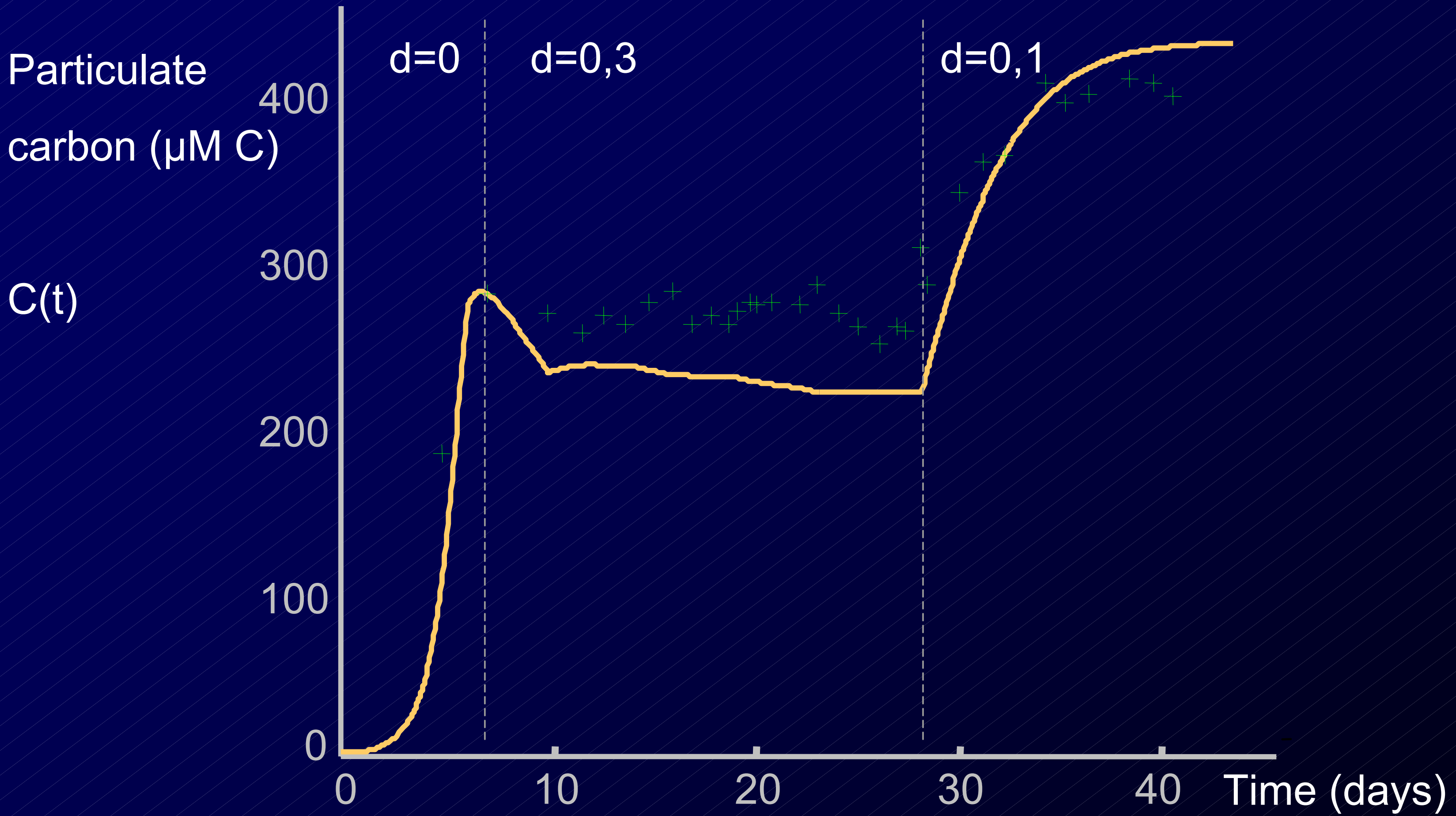
Steady state validation

Dynamical validation

Model vs. data



Model vs. data



→ Simulations are coherent with observations.

BioLOV : Further improvements

→ BioLOV outputs are coherent at steady-state with observations.

→ BioLOV provides additionnal outputs such as growth rate, quotas, net flux of carbon.

→A formulation with integration of temperature exists but has not been compared with observations.

→ Its behaviour for periodic light signals is currently under test. Qualitative behaviour is satisfying but chlorophyll and carbon are underestimated.

→ Processes independant with light (nitrate uptake, degradation, respiration) should be studied to see if light should be taken account in these processes.

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