Calibration of a biokinetic model to simulate microalgae growth

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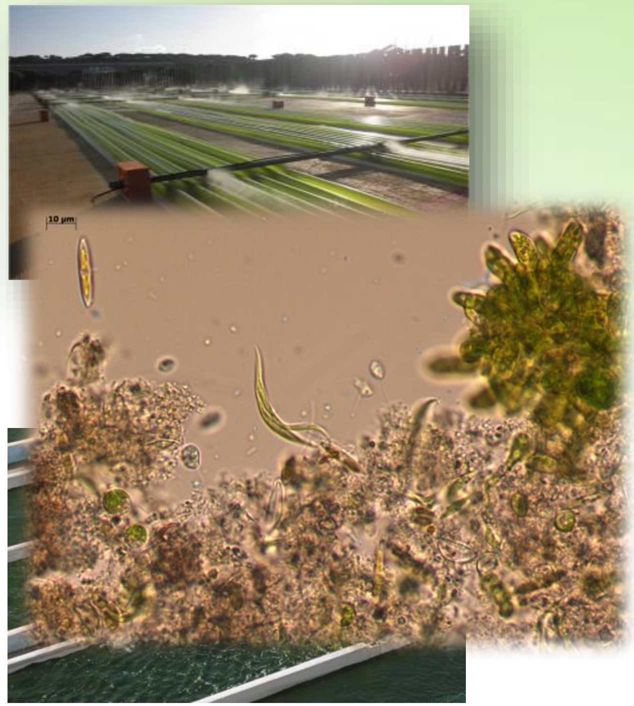
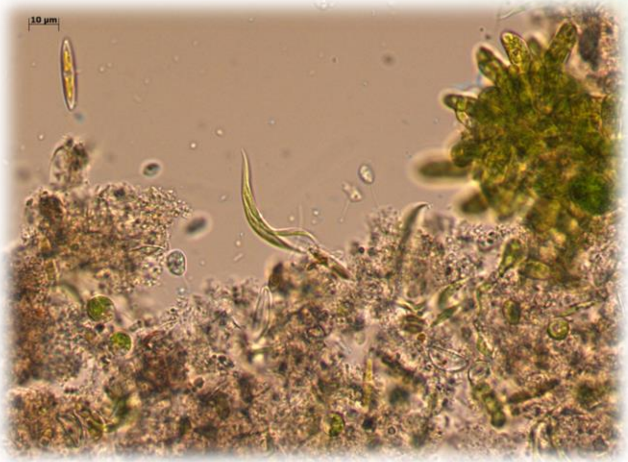
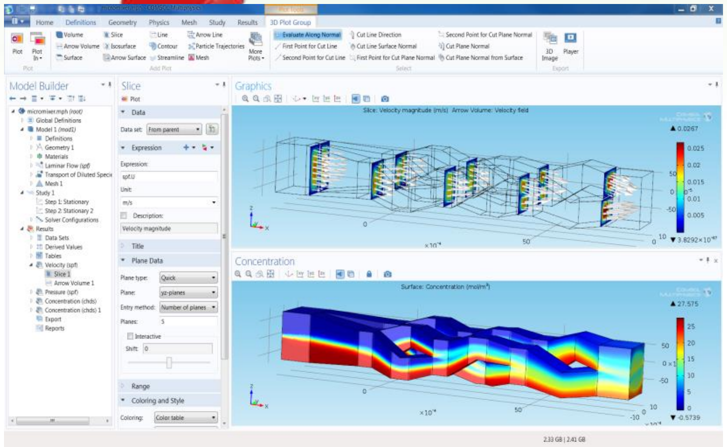


Introduction





Introduction

Objectives

- To show a new mechanistic model that includes physical and biokinetic processes to simulate microalgae growth in photobioreactors and open ponds
- To implement the mathematical model into Comsol Multiphysics to simulate the microalgae growth in different case studies.
- To calibrate the model using experimental data

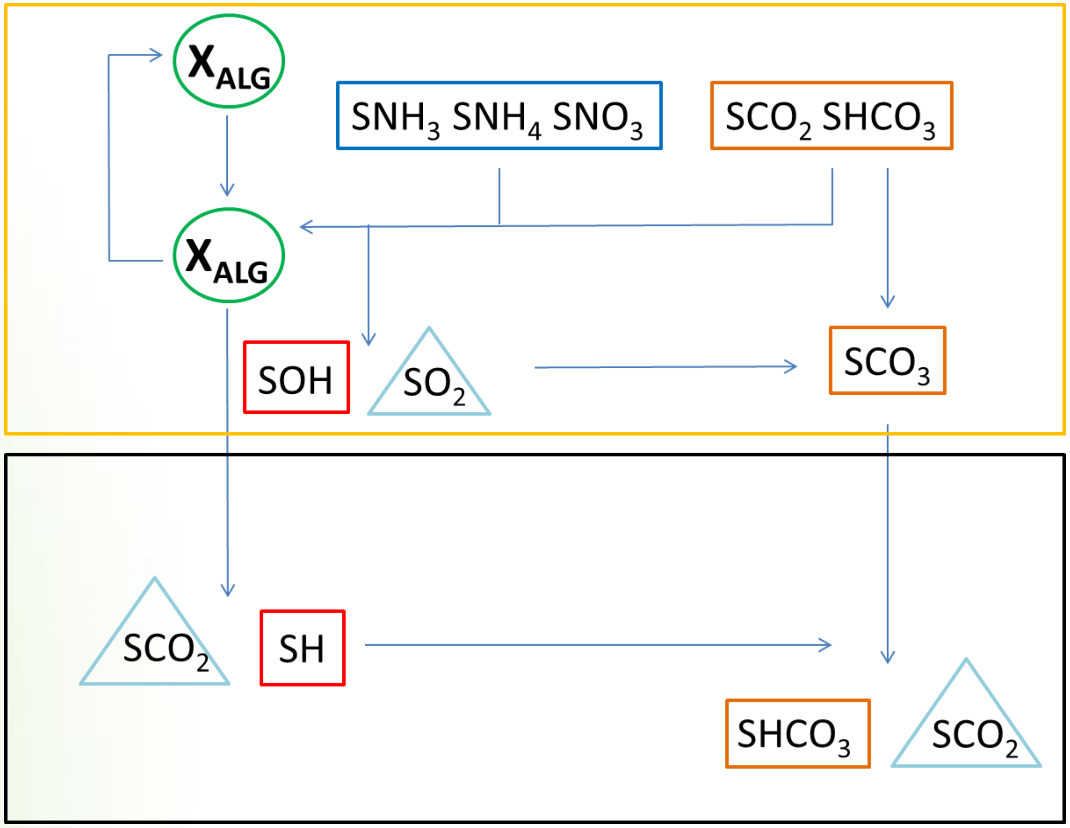
The Model

Physic and chemical processes mediated by microalgae

Biokinetic expressions of RWQM1

0_D domain

- Particulate component: X_{ALG}
- 9 Dissolved components: SNH_3 - SNH_4 – SNO_3 SCO_2 - SCO_3 - $SHCO_3$ SH – SOH - SO_2



Grow of microalgae, equilibrium process and photosynthesis and photoinhibition sub-model compose the structure of this model.

Processes	Mathematical equation
Growth of algae on NH_4	$\rho_{1a} = \mu_{ALG} \cdot f_{T,FS}(T) \cdot \eta_{PS}(I, S_{O2}) \cdot \frac{S_{CO2}+S_{HCO3}}{K_{C,ALG}+S_{CO2}+S_{HCO3}+\frac{S_{CO2}{}^2}{I_{CO2,ALG}}} \cdot \frac{S_{NH3}+S_{NH4}}{K_{N,ALG}+S_{NH3}+S_{NH4}} \cdot X_{ALG}$
Growth of algae on NO_3	$\rho_{1b} = \mu_{ALG} \cdot f_{T,FS}(T) \cdot \eta_{PS}(I, S_{O2}) \cdot \frac{S_{CO2}+S_{HCO3}}{K_{C,ALG}+S_{CO2}+S_{HCO3}+\frac{S_{CO2}{}^2}{I_{CO2,ALG}}} \cdot \frac{S_{NO3}}{K_{N,ALG}+S_{NO3}} \cdot \frac{K_{N,ALG}}{K_{N,ALG}+S_{NH3}+S_{NH4}} \cdot X_{ALG}$
Endogenous aerobic respiration	$\rho_2 = K_{resp,ALG} \cdot f_{T,FS}(T) \cdot \frac{S_{O2}}{K_{O2,ALG}+S_{O2}} \cdot X_{ALG}$
Inactivation of algae	$\rho_3 = K_{death,ALG} \cdot f_{T,FS}(T) \cdot X_{ALG}$
Chemical Equilibrium CO_2 - HCO_3^-	$\rho_{13} = k_{eq,1} \cdot (S_{CO2} - \frac{S_H S_{HCO3}}{K_{eq,1}})$
Chemical Equilibrium HCO_3^- - CO_3^{2-}	$\rho_{14} = k_{eq,2} \cdot (S_{HCO3} - \frac{S_H S_{CO3}}{K_{eq,2}})$
Chemical Equilibrium NH_4^+ - NH_3	$\rho_{15} = k_{eq,3} \cdot (S_{NH4} - \frac{S_H S_{NH3}}{K_{eq,3}})$
Chemical Equilibrium H^+ - OH^-	$\rho_{16} = k_{eq,w} \cdot (1 - \frac{S_H S_{OH}}{K_{eq,w}})$
Volatilization O_2	$\rho_{O2} = K_{O2}^{G-L} \cdot (S_{O2}^{AIR}(T) - S_{O2})$
Volatilization CO_2	$\rho_{CO2} = K_{CO2}^{G-L} \cdot (S_{CO2}^{AIR}(T) - S_{CO2})$
Volatilization NH_3	$\rho_{NH3} = K_{NH3}^{G-L} \cdot (-S_{NH3})$

The kinetic processes are described by Monod equation

$$\rho_{1a} = \mu_{ALG} * \frac{S_{CO2} + S_{HCO3}}{K_{C,ALG} + S_{CO2} + S_{HCO3} + \frac{S_{CO2}{}^{2}}{I_{CO2,ALG}}} * \frac{S_{NH3} + S_{NH4}}{K_{N,ALG} + S_{NH3} + S_{NH4}} * X_{ALG}$$

Maximum growth rate of microalgae

Carbon as a limiting factor and inhibitor at high concentrations

Nitrogen as a limiting factor

$f_{T,FS}(T)$ → Thermic photosynthetic factor

$\eta_{PS}(I, S_{O2})$ → Factor of photosynthetic performance

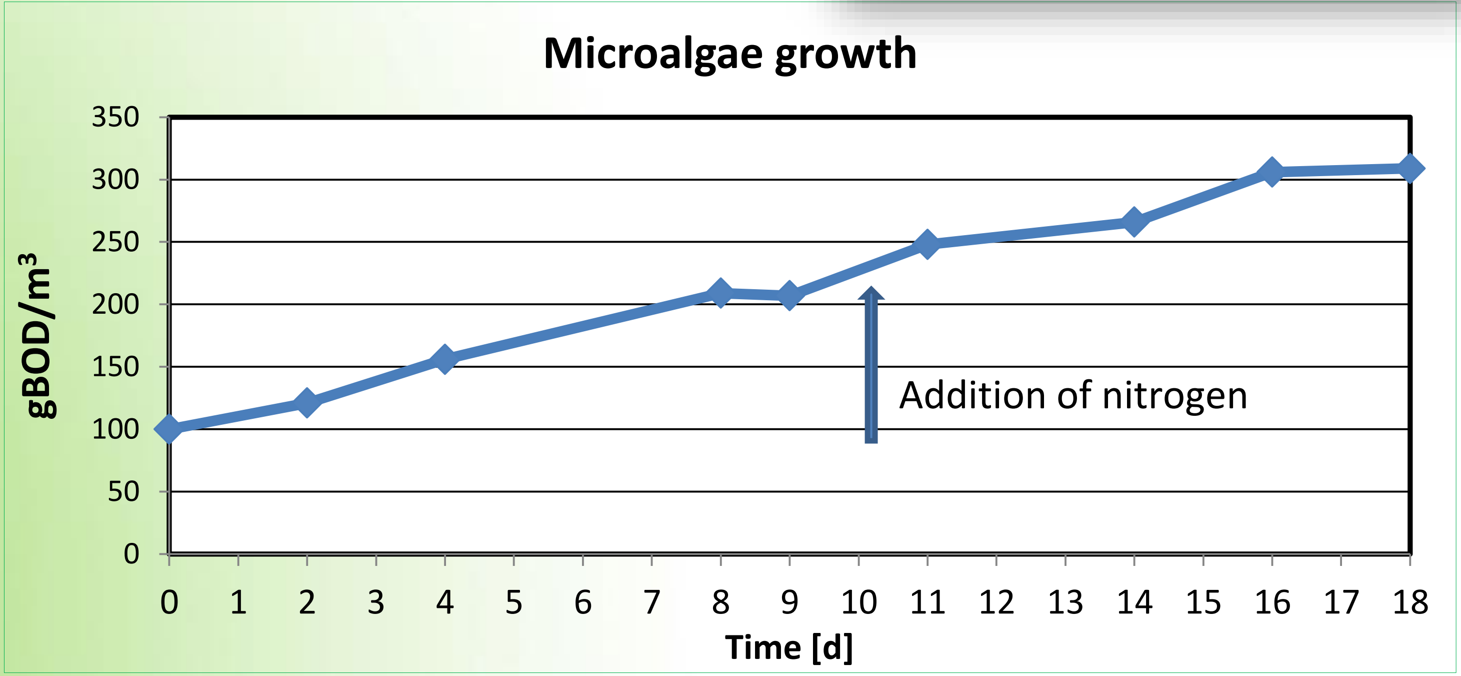
$$\eta_{PS}(I, S_{O2}) = f_L(I) * f_{PR}(S_{O2})$$

To evaluate algae growth or dissolved components concentration we have to sum the product of each process by its correponding stoichiometric coefficient

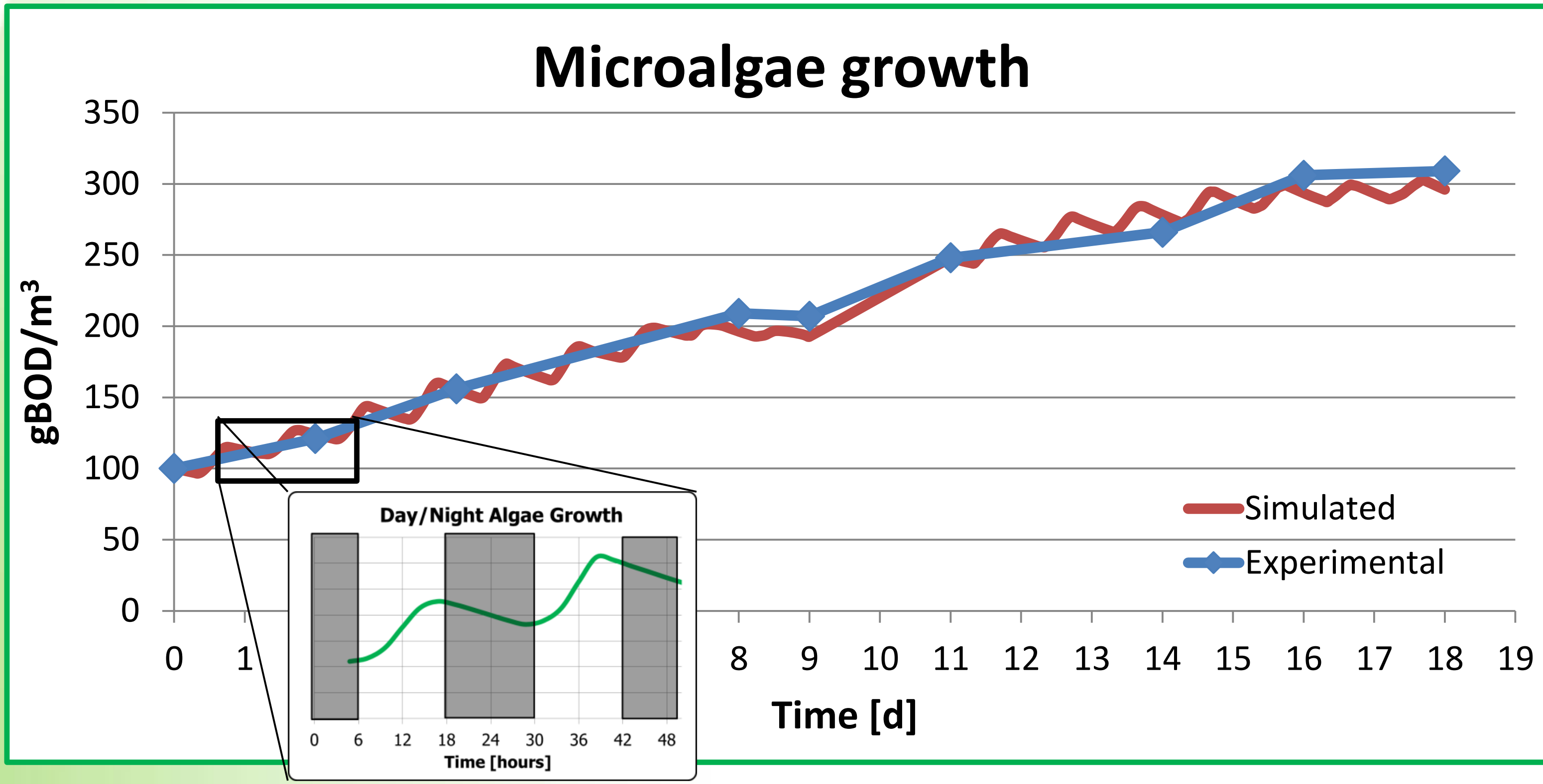
Processes/State variables	S_{NH4}	S_{NH3}	S_{NO3}	S_{O2}	S_{CO2}	S_{HCO3}	S_{CO3}	S_H	S_{OH}	X_{ALG}
Algae growth on SNH_4	$v_{3,1a}$			$v_{8,1a}$	$v_{9,1a}$			$v_{12,1a}$		$v_{14,1a}$
Algae growth on SNO_3			$v_{6,1b}$	$v_{8,1b}$	$v_{9,1b}$			$v_{12,1b}$		$v_{14,1b}$
End. Aerobic respiration	$v_{3,2}$			$v_{8,2}$	$v_{9,2}$			$v_{12,2}$		$v_{14,2}$
Inactivation of algae	$v_{3,3}$			$v_{8,3}$	$v_{9,3}$			$v_{12,3}$		$v_{14,3}$
Chemical eq. CO2- HCO_3^-					$v_{9,13}$	$v_{10,13}$		$v_{12,13}$		
Chemical eq. HCO_3^- - CO_3^{2-}						$v_{10,14}$	$v_{11,14}$	$v_{12,14}$		
Chemical eq. NH_4^+ - NH_3	$v_{3,15}$	$v_{4,15}$						$v_{12,15}$		
Chemical eq. H^+ - OH^-								$v_{12,16}$	$v_{13,16}$	
Volatilization of O_2				$v_{8,O2}$						
Volatilization of CO_2					$v_{9,CO2}$					
Volatilization of NH_3		$v_{4,NH}$								

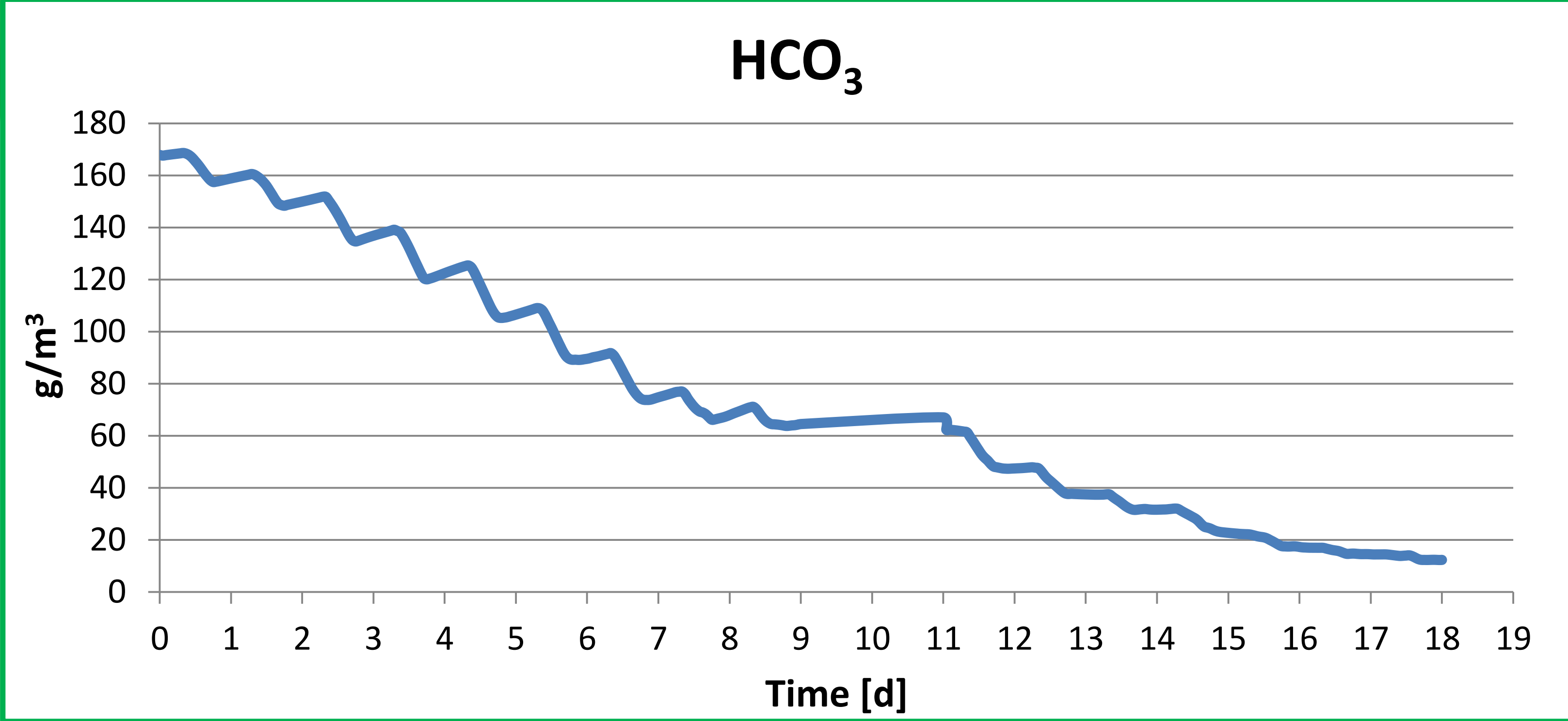
The model was calibrated through a case study based on cultivation of microalgae in a synthetic waste water.

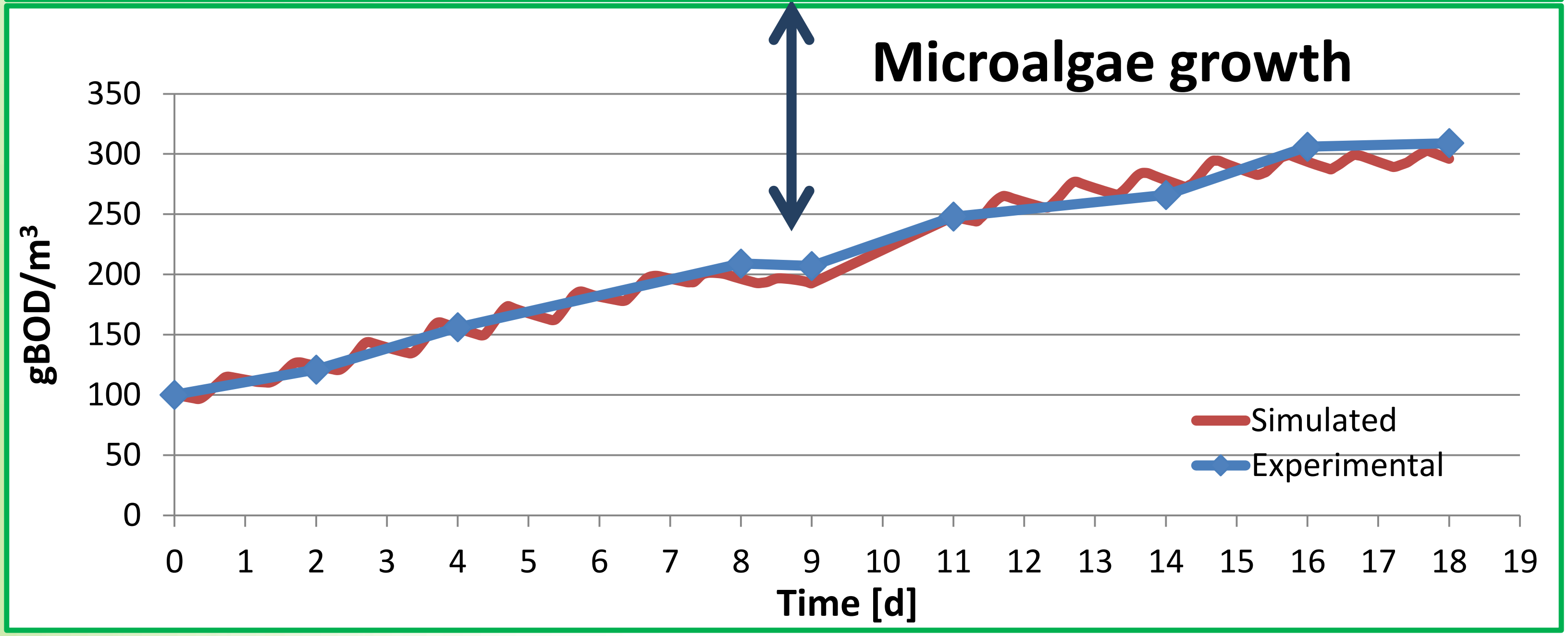
Parameter	Concentration	Units
TC	170	g/m^3
TN	8,3	g/m^3
pH	8,5	
X_{ALG}	100	$gBOD/m^3$



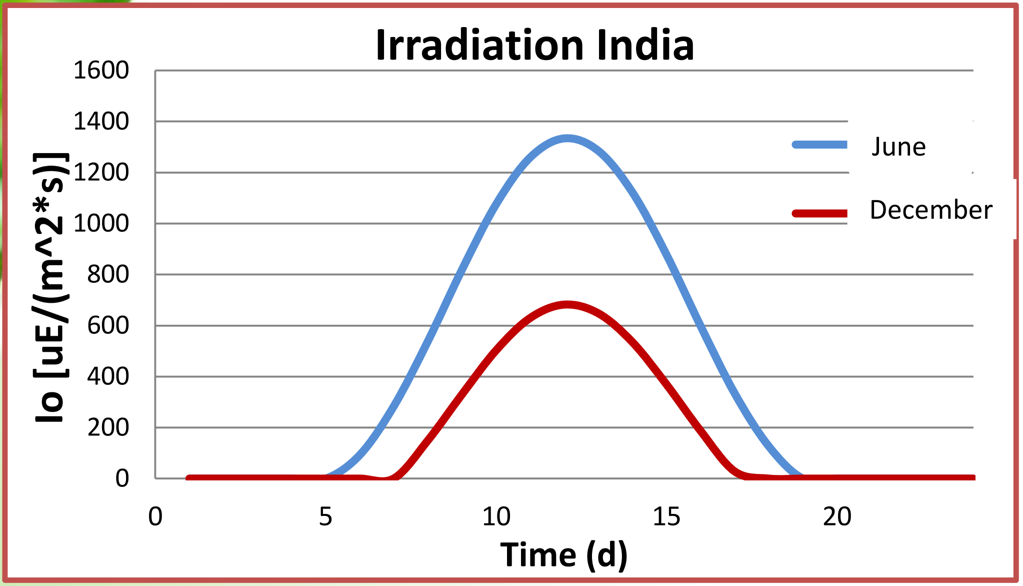
Parameter	Descrption	Value
μ_{ALG}	Maximum growth rate of algae	1,5 d^{-1}
K_{O2}	Mass transfer coefficient from O_2	20 d^{-1}

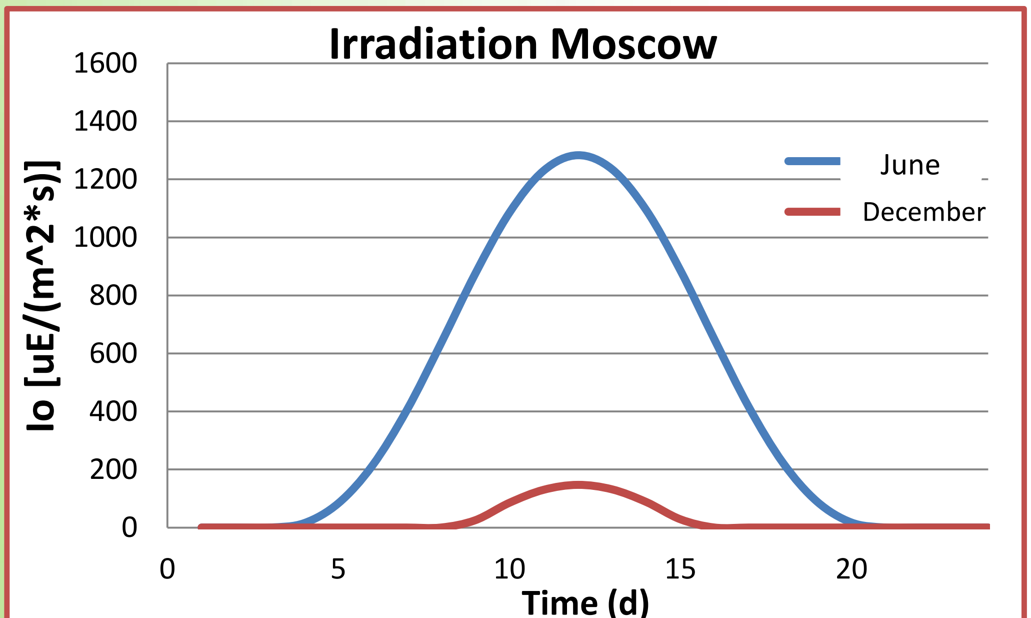



HCO3
g/m3
Time [d]


Microalgae growth
gBOD/m3
Time [d]
Simulated
Experimental

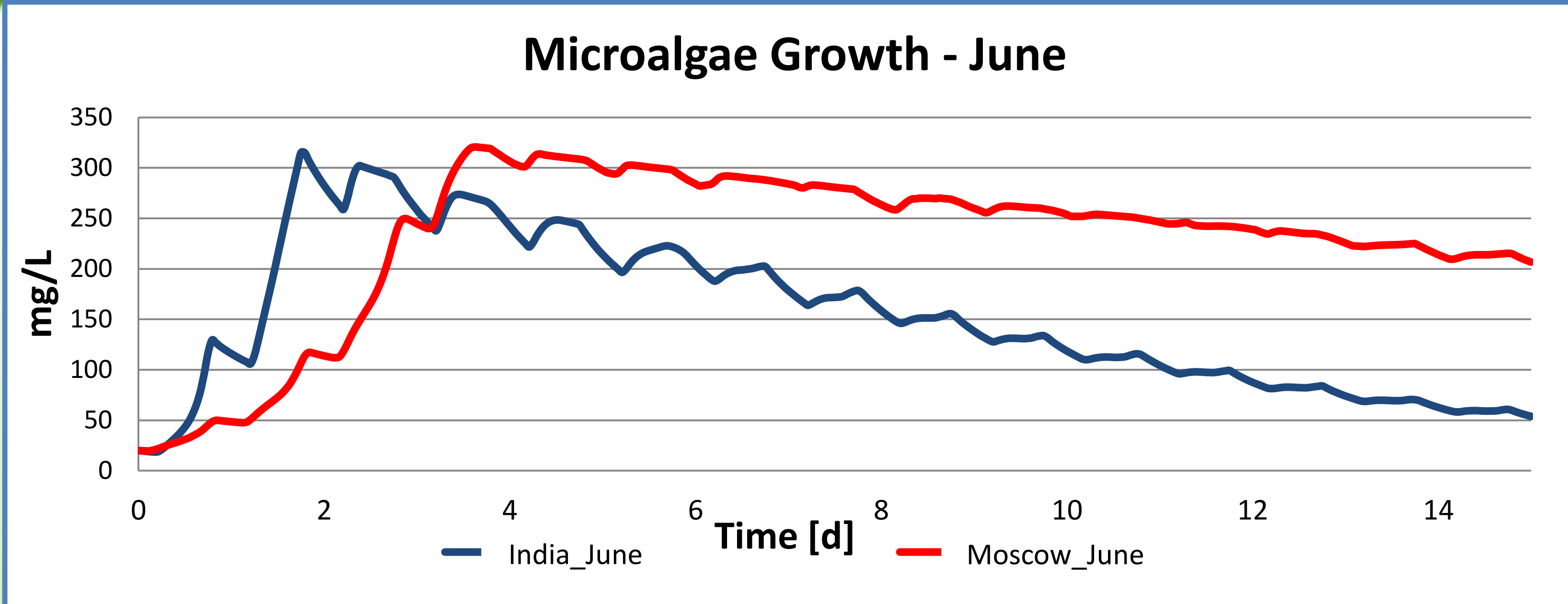
Case Study : effect of temperature and irradiation

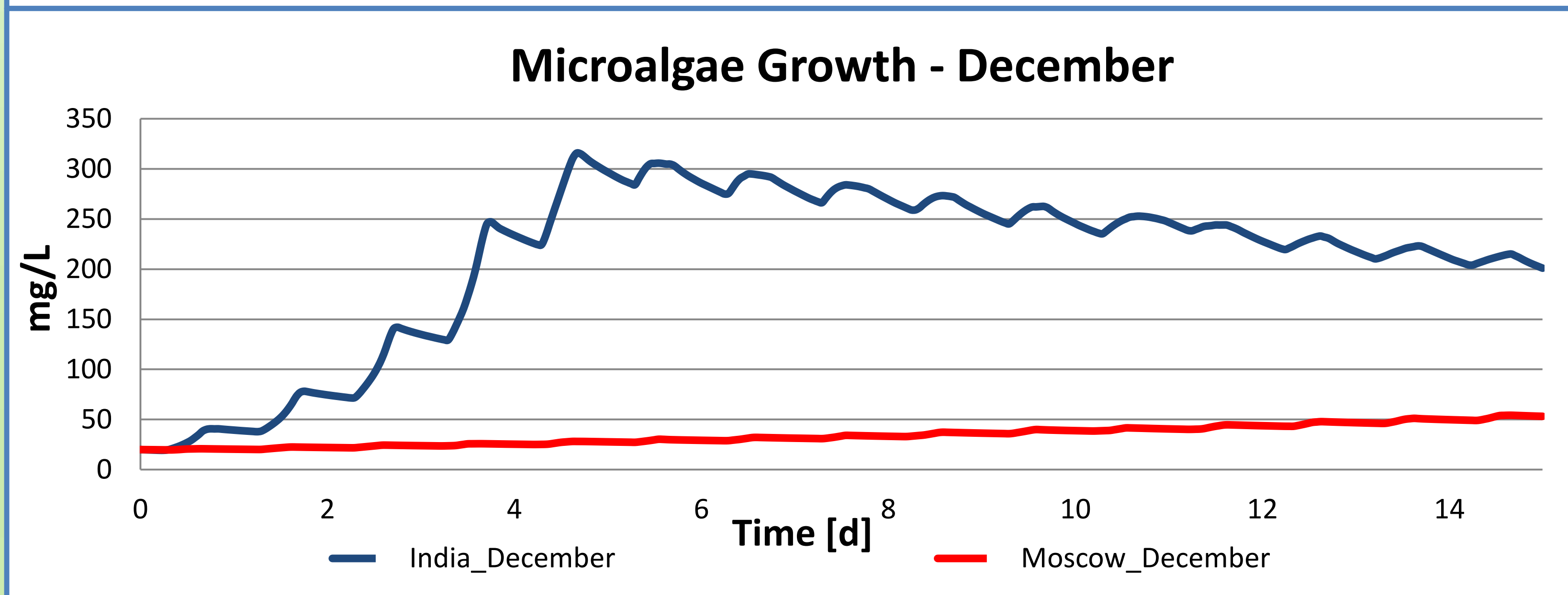




	Índia		Moscou	
Hora	June (ºC)	December (ºC)	June (ºC)	December (ºC)
0:00	39	19	16	-11
1:00	28	18	17	-10
2:00	37	17	18	-9
3:00	36	16	18	-9
4:00	35	15	18	-9
5:00	34	14	18	-9
6:00	33	13	18	-9
7:00	35	15	18	-9
8:00	37	17	18	-9
9:00	39	19	19	-8
10:00	41	21	20	-7
11:00	43	24	20	-7
12:00	44	25	21	-6
13:00	45	26	21	-6
14:00	46	27	21	-6
15:00	46	27	22	-5
16:00	46	27	22	-5
17:00	45	26	23	-4
18:00	45	26	22	-5
19:00	43	22	22	-5
20:00	42	21	21	-6
21:00	40	19	21	-6
22:00	40	19	20	-7
23:00	39	18	20	-7

Case Study : effect of temperature and irradiation





- Adopting RWQM1 as base model and considering the dissolved carbon as a limiting factor for the growth of microalgae, it has been possible to implement in COMSOL Multiphysics an integral biokinetic model.

- The model is able to accurately simulate the microalgae growth in the experiment.

- The next step will be to simulate the hydraulic and hydrodinamic behaviour in a photobioreactor and implent in the model the processes of bacteria

Thank you for attention!

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