

MSc CMEE PROJECT

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DEPARTMENT OF LIFE SCIENCE

Supplementary Information

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1 Cellular Automata theory

In the 1940s, John von Neumann and Stanislaw Ulam first proposed Cellular Automata, a system in which space and time are discrete and physical quantities take on a finite set of discrete values (Sarkar 2000). CAs consist of a grid of cells, each of which is in one of a finite number of states. The grid can have any number of finite dimensions. Time is also discrete, and the state of a cell at time t is determined by the states of neighbouring cells at time $t-1$, in accordance with a particular set of transition rules.

The most known cellular automata model application might be Conway's Game of Life (Bays 2010), a two-dimensional automaton in which cells can be in one of two states: "alive" or "dead". In this case, the transition rules determine whether a cell will be "alive" or "dead" in the next generation based on the number of "alive" cells in its eight-cell neighbourhoods in the current generation, for example, if a living cell has fewer than two living neighbours, it dies; or a deceased cell will be restored back to life if it is surrounded by exactly three living cells.

While the use of CA theory in this project is more complex and detailed, this simplified example illustrates the fundamental principles underlying all cellular automata. Similar to Conway's Game of Life, this seagrass restoration model will rely on local rules to determine global behaviour. However, the local norms and the resulting global behaviour were tailored to the particular research questions which intend to answer in this project. The following sections describe the construction of the internal dynamic ecological model in this CA to encapsulate and investigate the complexities of this research topic.

2 Ecological models

Fundamental to these ecological models are the dynamic models developed by Italian scientists Elisabetta Giusti and Stefano Marsili-Libelli, as detailed in their paper titled "Modelling the interactions between nutrients and the submersed vegetation in the Orbetello Lagoon" (Giusti and Marsili-Libelli 2005; Giusti and Marsili-Libelli 2006).

2.1 Nitrogen Dynamics

The nitrogen (N) cycle, vital in aquatic ecosystems, intricately intertwines with various forms of nitrogen including organic nitrogen, ammonia, nitrite, and nitrate. In this N model (Giusti and Marsili-Libelli 2005), we delve deep into the temporal evolution of these nitrogen forms, emphasizing their dynamic interactions within the seagrass environment and their susceptibility to factors such as seagrass growth rate, temperature, and water column height.

The dynamics of nitrogen in the water column can be categorized by specific state variables. Particulate organic-N (N_{org}) is either sourced from external inputs or released during the decomposition of detritus. Ammonium-N (NH_4^+), on the other hand, emerges from ammonification processes, direct release from detritus, or other anthropogenic sources. In environments characterized by elevated pH levels, a substantial fraction of ammonium-N transitions to ammonia. This ammonia, depending on the pH and water temperature, can either remain in the water or be volatilized as gaseous NH_3 , which is lost to the atmosphere. Such conversion and potential loss are pivotal for the nitrogen balance in the water, especially given ammonia's inherent toxicity. Moreover, through biological oxidation, ammonium-N is first transformed to nitrite-N (NO_2^-) and then to nitrate-N (NO_3^-) (Zimmo et al. 2003). It's also noteworthy that regions with dense macroalgal growth often exhibit heightened ammonium concentrations, a direct result of the decomposition of senescent macroalgal tissue.

To provide a structured understanding of these dynamics, we articulated the associated model equations in Table 1. These equations, derived and adapted from previous research, serve as the mathematical backbone for our model, offering quantifiable insights into the interplay of the various nitrogen forms.

2.2 Phosphorus Dynamics

In tandem with the investigation of the nitrogen dynamics, the phosphorus dynamics inherent to seagrass ecosystems are also modelled. Multiple forms of phosphorus, including Phosphorus in Organic Particulates, Soluble Reactive Phosphorus, and internal phosphorus reservoirs in both macroalgae and seagrass, are incorporated into the phosphorus cycle in this context.

In the past research, even in the early seagrass growth model that proposed by Giusti and Marsili-Libelli (2005), considered only nitrogen as the pivotal nutrient. However, relying solely on this approach tends to simplify the complex interplay within these ecosystems. Recent research highlights both a significant phosphorus scarcity and the dominance of nitrophilous species. The sediment, acting as a major nutrient storehouse, is crucial in this context. Its oxidation level largely influences macroalgae variety and quantity. It's worth noting that alterations in these sediment conditions, like those seen in the 1990s, can cause a shift towards species adapted to phosphorus-poor environments (Giusti and Marsili-Libelli 2006).

This phosphorus model is underpinned by two key variables: Soluble Reactive Phosphorus (SRP) and Particulate Organic Phosphorus (POP). While SRP represents a dissolved nutrient component directly assimilated by vegetation, POP typifies a detritus component on the surface that undergoes decomposition in the upper sediment layers. The development of this phosphorus model took cues from the foundational guidelines of our nitrogen model. We've modelled storage and uptake rates using Michaelis–Menten terms, reflecting cellular requirements and associated internal storage mechanisms. The release of phosphorus from sediment is also intricately modelled, mirroring the methodology employed for nitrogen.

The newly introduced equations, which encapsulate algal uptake, sediment fluxes, and organic matter mineralization, are systematically delineated in Table 2.

2.3 Growth Dynamics

This simulation employs a set of ordinary differential equations (ODEs) to model seagrass growth. This approach considers the uptake of nitrogen and the corresponding growth rate of the seagrass, factoring in environmental and physiological parameters like nitrogen concentration, temperature, and light conditions.

3 Parameters Selection and Input Data

For the initial parameter values used in this study, please refer to Table 4 in this SI document. This table provides an overview of the parameters and their corresponding initial values, which serve as a foundation for the model's calculations.

4 Computing Tools

Python (version 3.9.12, Van Rossum and Drake 2009) was used to develop and analyze this seagrass ecosystem model. For better modification and management of the model, the complete model was separated into modular sub-models. Packages *NumPy* Harris et al. 2020, *SciPy* Virtanen et al. 2020, and *Matplotlib* (version 3.5.2, Hunter 2007) were used throughout the project due to their ease of use for data frame manipulation, mathematical operations, and efficient visualizations. R (version 4.2.1, R Core Team 2022) packages *dplyr* Wickham et al. 2022 and *ggplot2* Wickham 2016, known for providing high-quality data visualizations with concise code, were used for plotting and results analysis. Bash (version 3.2, GNU 2007) was used to execute project scripts, capture outputs, and compile LaTeX (version 3.141592653-2.6-1.40.24 (TeX Live 2022)) documents.

Parameter	Unit	Value	Description	References/remarks
a	NaN	20.0000	Ruppia light limitation coefficient	Giusti and Marsili-Libelli (2005)
b	NaN	2.0000	Ruppia light limitation coefficient	Giusti and Marsili-Libelli (2005)
c	NaN	5.0000	Ruppia temperature limitation coefficient	Giusti and Marsili-Libelli (2005)
d	NaN	2.0000	Ruppia temperature limitation coefficient	Giusti and Marsili-Libelli (2005)
f_o	h	14.0000	Ruppia maximum growth photoperiod	Calado and Duarte (2000)
f_v	m ³ /L	0.0010	Dimensional conversion factor	NaN
k_1	NaN	0.3000	Temperature adjustment coefficient	Bendoricchio et al. (1994)
k_4	NaN	0.0100	Temperature adjustment coefficient	Bendoricchio et al. (1994)
k_AP	/day	0.0430	Anaerobic POP mineralization rate	Calibrated
k_I	kcal/m ² /day	242.0000	Photosynthesis half saturation constant	Chapelle (1995) and Calado and Duarte (2000)
k_oo	/m	0.4000	Light extinction coefficient	Coffaro and Bocci (1997)
k_op	mg*O ₂ /L	4.4500	DO half-saturation constant for POP mineralization	Calibrated
kP_ma	mg*N*g/dw	0.0061	MacroalgaeSRPhalf-saturationconstant	Calibrated
kP_R	mg*N*g/dw	0.0115	Ruppia SRP half-saturation constant	Calibrated
K_tox	/°C	3.0000	Toxic mortality adjustment coefficient	Coffaro and Bocci (1997)
N_min	mg*N*g/dw	10.0000	Ruppia minimum internal N quota	Coffaro and Bocci (1997)
N_cri	mg*N*g/dw	15.0000	Ruppia critical internal N quota	Coffaro and Bocci (1997)
P_SRP	mg*m ² /day	13.7000	Sediment SRP release rate	Hu et al. (2001)
QN_min	mg*N*g/dw	10.0000	Macroalgae minimum intracellular N quota	Coffaro and Bocci (1997)
QN_max	mg*N*g/dw	40.0000	Macroalgae maximum intracellular N quota	Coffaro and Bocci (1997)
QP_ma_max	mg*g/dw	3.9000	Macroalgae maximum intracellular P quota	Giovanni Coffaro and Sfriso (1997)
QP_ma_min	mg*g/dw	1.1000	Macroalgae minimum intracellular P quota	Giovanni Coffaro and Sfriso (1997)
QP_R_max	mg*g/dw	1.2000	Ruppia maximum intracellular P quota	Touchette and Burkholder (2000)
QP_R_min	mg*g/dw	0.7000	Ruppia minimum intracellular P quota	Touchette and Burkholder (2000)
R_max	g*dw/m ²	250.0000	Ruppia maximum shoot biomass	Coffaro and Bocci (1997)
SL	g*dw/m ²	5.0000	Ruppia growth dependence on space availability	Coffaro and Bocci (1997)
SR	/day	0.0800	Ruppia decay rate	Calibrated
T_max	°C	26.0000	Maximum temperature	Bendoricchio et al. (1994)
T_min	°C	8.0000	Minimum temperature	Bendoricchio et al. (1994)
T_o	°C	26.0000	Ruppia optimum temperature	Calado and Duarte (2000)
T_opt	°C	24.0000	Optimum temperature	Bendoricchio et al. (1994)

Continued on next page

Parameter	Unit	Value	Description	References/remarks
tox	/day	0.1100	Toxic mortality rate	Coffaro and Bocci (1997)
Ulv_ext	g/dw	0.0010	Macroalgae light extinction	Giovanni Coffaro and Sfriso (1997)
vP_ma_max	mg*P*g/dw	0.2000	Macroalgae maximum SRP uptake rate	Romero et al. (2004)
vP_R_max	mg*P*g/dw	0.1000	Ruppia maximum SRP uptake rate	Romero et al. (2004)
alpha_P_ma	mg*P*g/dw	0.2300	Macroalgae detritus P content	Lenzi et al. (2003)
alpha_P_R	mg*P*g/dw	0.1100	Ruppia detritus P content	Lenzi et al. (2003)
mu_max	/day	0.3700	Macroalgae maximum growth rate	Calibrated
rho_max	/day	0.2300	Ruppia maximum growth rate	Calibrated
omega_m	/day	0.0400	Macroalgae decay rate	Calibrated

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Table 2: Nitrogen submodel from Giusti and Marsili-Libelli (2005)

Explanation	Model Equation	Number
Organic-N dynamics	$\frac{dN_{\text{org}}}{dt} = f_v \psi_{a1} f_{\text{deta}1} \frac{\Omega_{ma} B}{h} + f_v \psi_{a2} f_{\text{deta}2} \frac{\Omega_R R}{h} - \mu_{\text{max}04} N_{\text{org}}$	(1)
Ammonium-N dynamics	$\frac{d\text{NH}_4}{dt} = \mu_{\text{max}04} N_{\text{org}} + \delta_{\text{rsed}4} - \text{up}_{\text{NH}4a1} - \text{up}_{\text{NH}4a2} - \mu_{\text{max}42} \frac{\text{DO}}{\text{DO} + K_O} \theta^{(T-20)} \text{NH}_4$	(2)
Ammonium-N uptake rates for cell quota	$\text{up}_{\text{NH}4a1} = \frac{B}{h} v_{\text{NH}}^{ma} \frac{\text{NH}_4}{\text{NH}_4 + K_{\text{NH}}} \frac{N_{\text{int}} - Q N_{\text{min}}}{Q N_{\text{max}} - Q N_{\text{min}}} f_v$ $\text{up}_{\text{NH}4a2} = \frac{R}{h} v_{\text{NH}_4}^R \frac{\text{NH}_4}{\text{NH}_4 + K_{\text{NH}_4}} f_v$	(3)
Nitrite-N dynamics	$\frac{d\text{NO}_2}{dt} = \mu_{\text{max}42} \frac{\text{DO}}{\text{DO} + K_O} \theta^{(T-20)} \text{NH}_4 - \mu_{\text{max}23} \frac{\text{DO}}{\text{DO} + K_O} \theta^{(T-20)} \text{NO}_2$	(4)
Nitrate-N dynamics	$\frac{d\text{NO}_3}{dt} = \mu_{\text{max}23} \frac{\text{DO}}{\text{DO} + K_O} \theta^{(T-20)} \text{NO}_2 - \mu_{\text{denit}} \frac{K_{O3}}{\text{DO} + K_{O3}} \theta^{(T-20)} \text{NO}_3 - \text{up}_{\text{NO}3a1} - \text{up}_{\text{NO}3a2} + \delta_{\text{rsed}3}$	(5)
Nitrate-N uptake rates for cell quota	$\text{up}_{\text{NO}3a1} = \frac{B}{h} v_{\text{NO}}^{ma} \frac{\text{NO}_3}{\text{NO}_3 + K_{\text{NO}}} \frac{N_{\text{int}} - Q N_{\text{min}}}{Q N_{\text{max}} - Q N_{\text{min}}} f_v$ $\text{up}_{\text{NO}3a2} = \frac{R}{h} v_{\text{NO}_3}^R \frac{\text{NO}_3}{\text{NO}_3 + K_{\text{NO}_3}} f_v$	(6)

Table 3: Phosphorus submodel from Giusti and Marsili-Libelli (2006)

Variable/process	Equation	Number
POP, particulate organic phosphorus	$\frac{dPOP}{dt} = \left(\frac{k_{AP}k_{QP}+k_{PO}DO}{k_{OP}+DO} \right) \cdot f(T) \cdot POP + a_{ma}^P \cdot B \cdot \Omega_{ma} + a_R^P \cdot R \cdot \Omega_R$	(7)
SRP, soluble reactive phosphorus	$\frac{dSRP}{dt} = \left(\frac{k_{AP}k_{QP}+k_{PO}DO}{k_{OP}+DO} \right) \cdot f(T) \cdot POP + \delta_{rsed-P} - \text{uptake}_R - \text{uptake}_{ma}$	(8)
P_{int}^{ma} , Macroalgae internal phosphorus storage	$\frac{dP_{int}^{ma}}{dt} = v_{P_{ma}(max)} \cdot \frac{SRP}{SRP+k_{P_{ma}}} \cdot \frac{Q_{P_{max}}^{ma}-P_{int}^{ma}}{Q_{P_{max}}^{ma}-Q_{P_{min}}^{ma}} - \mu_{ma} \cdot P_{int}^{ma}$	(9)
P_{int}^R , Seagrass internal phosphorus storage	$\frac{dP_{int}^R}{dt} = v_{P_R(max)} \cdot \frac{SRP}{SRP+k_{P_R}} \cdot \frac{Q_{P_{max}}^R-P_{int}^R}{Q_{P_{max}}^R-Q_{P_{min}}^R} - \rho \cdot P_{int}^R$	(10)
Sediment release of phosphorus	$\delta_{rsed-P} = \begin{cases} -\frac{P_{SRP}}{\pi} \cdot \tan^{-1} \left(\frac{ORP_s}{4} \right) + \frac{P_{SRP}}{2}, & ORP_s \leq 0 \\ e^{-(ORP_s - \frac{P_{SRP}}{2})}, & ORP_s > 0 \end{cases}$	(11)
Macroalgae and Seagrass phosphorus uptake	$\begin{aligned} \text{uptake}_{ma} &= \frac{B}{h} \cdot v_{P_{ma}(max)} \cdot \frac{SRP}{SRP+k_{P_{ma}}} \cdot \frac{Q_{P_{max}}^{ma}-P_{int}^{ma}}{Q_{P_{max}}^{ma}-Q_{P_{min}}^{ma}} \cdot f_v \\ \text{uptake}_R &= \frac{R}{h} \cdot v_{P_R(max)} \cdot \frac{SRP}{SRP+k_{P_R}} \cdot \frac{Q_{P_{max}}^R+P_{int}^R}{Q_{P_{max}}^R-Q_{P_{min}}^R} \cdot f_v \end{aligned}$	(12)
Macroalgae dynamics	$\begin{aligned} \frac{dB}{dt} &= (\mu_{ma} - \Omega_{ma}) \cdot B \\ \mu_{ma} &= \mu_{max} \cdot f_{ma}(I) \cdot f_{ma}(T) \cdot f_{ma}(N_{int}^{ma}) \cdot f_{ma}(P_{int}^{ma}) \\ \Omega_{ma} &= \Omega_m + \text{tox} \cdot e^{K_{tox}(T-26)} \\ f_{ma}(P_{int}^{ma}) &= \frac{Q_{P_{max}}^{ma}-P_{int}^{ma}}{Q_{P_{max}}^{ma}-Q_{P_{min}}^{ma}} \\ f_{ma}(I) &= \frac{1}{K_{ext} \cdot h} \cdot \ln \left(\frac{K_I+I}{K_I+I \cdot e^{-K_{exp} \cdot h}} \right) \text{ with } K_{ext} = K_{OO} + U_{IV_{ext}} \cdot \frac{B}{h} \\ f_{ma}(T) &= \frac{k_1 \cdot \exp(\gamma_1 \cdot (T-T_{min}))}{1+k_1 \cdot (\exp(\gamma_1 \cdot (T-T_{min}))-1)} \cdot \frac{k_4 \cdot \exp(\gamma_2 \cdot (T-T_{min}))}{1+k_4 \cdot (\exp(\gamma_2 \cdot (T-T_{min}))-1)} \\ \gamma_1 &= \frac{1}{T_{opt}-T_{min}} \cdot \ln \left(\frac{0.98 \cdot (1-k_1)}{0.02 \cdot k_1} \right) \\ \gamma_2 &= \frac{1}{T_{max}-T_{min}} \cdot \ln \left(\frac{0.98 \cdot (1-k_4)}{0.02 \cdot k_4} \right) \\ f_{ma}(N_{int}^{ma}) &= \frac{N_{int}^{ma}-Q_{N_{min}}}{Q_{N_{max}}-Q_{N_{min}}} \end{aligned}$	(13)
Seagrass dynamics	$\begin{aligned} \frac{dR}{dt} &= (\rho - \Omega_R) \cdot R \\ \rho &= \rho_{max} \cdot g(d) \cdot f_R(T) \cdot f_R(R) \cdot f_R(N_{int}^R) \cdot f_R(P_{int}^R) \\ \Omega_R &= SR \times (0.098 + e^{-6.59+0.2217 \cdot T}) \\ g(d) &= 1 - \frac{1}{1+b \cdot e^{a(d-f_o)}} \\ f_R(T) &= \frac{1}{1+\left(\frac{T-T_0}{c}\right)^2} \\ f_R(R) &= 1 - e^{-(R-R_{max})/SL} \\ f_R(P_{int}^R) &= \frac{Q_{P_{max}}^R-P_{int}^R}{Q_{P_{max}}^R-Q_{P_{min}}^R} \\ f_R(N_{int}^R) &= \frac{N_{int}^R-N_{min}}{N_{cri}-N_{min}} \end{aligned}$	(14)

Table 4: Seagrass Dynamic from Giusti and Marsili-Libelli (2005)

Variable	Model equation	Number
Seagrass biomass Dynamics	$\frac{dR}{dt} = (\rho - \Omega_R) \cdot R$	(15)
Nitrogen cell quota kinetics	$\frac{dN_{\text{int}}^R}{dt} = v_{\text{NH}_4}^R \cdot \frac{\text{NH}_4}{\text{NH}_4 + K_{\text{NH}_4}} + v_{\text{NO}_3}^R \cdot \frac{\text{NO}_3}{\text{NO}_3 + K_{\text{NO}_3}} - \rho_N \cdot N_{\text{int}}^R$	(16)
Seagrass specific growth rate	$\rho = \rho_{\text{max}} \cdot g(d) \cdot f_R(T) \cdot f_r(N_{\text{int}}^R) \cdot f_R(R)$	(17)
Photoperiod function for growth rate	$g(d) = 1 - \frac{1}{1 + b \cdot e^{a(d-f_0)}}$	(18)
Temperature function for growth rate	$f_R(T) = \frac{1}{1 + \left(\frac{T - T_{\text{opt}}}{c}\right)^2}^d$	(19)
Density function for growth rate	$f(R) = 1 - e^{-(R - R_{\text{max}})/SL}$	(20)
Nitrogen cell quota limiting function	$f(N_{\text{int}}^R) = \frac{N_{\text{int}}^R - N_{\text{min}}}{N_{\text{cri}} - N_{\text{min}}}$	(21)
Seagrass decay rate	$\Omega_R = SR \times (0.098 + e^{-6.59 + 0.2217T})$	(22)

Table 5: Unknown Parameters

Parameter	Unit	Value	Description
k_PO	NaN	NaN	NaN
DO	NaN	NaN	Guess to be the value of Dissolved Oxygen
f_T	NaN	NaN	Guess to be the value of f_ma_T or f_R_T
T	NaN	NaN	real temperature
B	NaN	NaN	biomass for macroalgae
R	NaN	NaN	biomass for seagrass
h	m	-2.0	water colum height, guess could be change to wa...
I	NaN	NaN	likely be the light intensity, varies by time o...
J_resed4	NaN	NaN	NaN
J_resed3	NaN	NaN	NaN

Table 6: Constants Variables

Parameter	Description
P_ma_int	initial P value for macroalgae
P_R_int	initial P value for seagrass
ORP_s	NaN
N_ma_int	initial Ni value for macroalgae
N_R_int	initial Ni value for seagrass
v_R_NH	initial NH4 value for seagrass
v_ma_NH	initial NH4 value for macroalgae
N_int	initial Ni value
v_ma_NO	initial NO3 value for macroalgae
v_R_NO3	initial NO3 value for seagrass
the initial situation	N_org, NH4, NO2, NO3 for Ni_model; POP, SRP, P_ma_int, P_R_int from P_model