Ecophysiological Models in Simulations of an Aquatic Habitat for Closed-Loop Life Support Research

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A limitation in closed-loop life support system research is the no-availability of small-scale experimental capacities that may help to better understand the challenges in system closure, integration, and control. Ground-based aquatic habitats are an option for small-scale research relevant to bioregenerative life support systems (BLSS), given that they can operate as self-contained systems enclosing a habitat composed of various species in a single volume of water. This paper elaborates on the modeling, design, and simulation of a reconfigurable aquatic habitat for experiments in BLSS and automation. It focuses in the process of respiration: higher plants of the species *Bacopa Monnieri* produce O$_2$ for snails of the genus *Pomacea*. The snails consume the O$_2$ and generate CO$_2$, which is used by the plants in combination with radiant energy to generate O$_2$ through the process of photosynthesis. The paper expands the description of biological processes by introducing models of ecophysiological phenomena of the organisms involved. The model of the plants include a description of the rate of CO$_2$ assimilation as a function of irradiance. The snails instead are modeled through their rate of consumption, treated as a combination of a constant and a random variable to account for changes in metabolic rates and aestivation. The latter consists in brief periods of torpor of the metabolism of the snails in which oxygen consumption is considerably reduced. Simulations and validation runs with hardware show how these phenomena may act as disturbances for the control mechanisms that aim to maintain safe concentration levels of dissolved oxygen in the habitat.

I. Introduction

Long duration human spaceflight poses challenges for spacecraft autonomy and the regeneration of life support consumables, such as oxygen and water. Bioregenerative life support systems (BLSS), which make use of biological processes to transform biological by-products back into consumables, have the ability to recycle organic byproducts and are the preferred option for food production. This paper elaborates on the use of aquatic habitats as small-scale platforms for life support research. Aquaria involve biological processes, such as photosynthesis, that regenerate life support resources, such as oxygen. Their reuse of a limited volume of water, their opportunity for isolation from the atmosphere, and their capacity to support life forms make them a candidate for the study of closed-loop LSS. This paper focuses on the process of respiration in aquatic habitats: higher plants of the species *Bacopa Monnieri* produce O$_2$ for snails of the genus *Pomacea*. The snails consume the O$_2$ and generate CO$_2$, which is used by the plants in combination with radiant energy to generate O$_2$ through the process of photosynthesis. The paper expands the description of the biological processes by introducing ecophysiological models of the organisms involved. The model of the plants include a description of the rate of CO$_2$ assimilation as a function of irradiance. The snails instead are modeled through their rate of consumption, treated as a combination of a constant and a random variable to account for changes in metabolic rates and aestivation. The latter consists in brief periods of torpor of the metabolism of the snails in which oxygen consumption is considerably reduced. Simulations and validation runs with hardware show how these phenomena may act as disturbances for the control mechanisms that aim to maintain safe concentration levels of dissolved oxygen in the habitat.

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A. Background

Previous projects have made use of aquatic habitats for experiments in zoology and physiology in low Earth orbit (LEO), and for ecotoxicological studies in ground-based hardware. Results obtained with the Closed Equilibrated Biological Aquatic System (CEBAS) minimodule in Space Shuttle missions STS-89 and STS-90 show that microgravity does not affect aquatic habitats considerably for exposure periods of up to 16 days. This module also flew in STS-107, but no results were reported due to the accident of the Space Shuttle Columbia. Researchers from the Chinese Academy of Sciences have employed a Closed Aquatic Ecosystem (CAES) as well for experiments relevant to ecophysiology, a discipline that “seeks to clarify the role and importance of physiological processes in ecological relations of species.” A recent initiative by the Japanese Aerospace Exploration Agency (JAXA) plans to include an aquatic habitat in their International Space Station module, Kibo. Beyond these efforts, very little has been done to make use of aquatic habitats for research on spaceflight life support control and automation.

B. Preliminary Description

Experiments with the aquatic habitat focus on the process of respiration, in which $\text{O}_2$ is consumed by 15 snails of the genus *Pomacea* while exhaling $\text{CO}_2$ as a byproduct. Plants of the species *Bacopa Monnieri* regulate the concentration of $\text{CO}_2$ through photosynthesis, enabled by a 6-LED lamp of 300 [lm] and 90° view angle, producing the oxygen needed by snails and bacteria while aiming to maintain acceptable concentration levels in the habitat. Water serves as the medium in which these quantities are stored (dissolved), and through which they are exchanged between the organisms. The habitat consists of a 10-gallon tank divided in four compartments by three separators, as shown in Figure 1; the first two with an opening area of 12.60 [$\text{cm}^2$] and the third with 48.00 [$\text{cm}^2$]. Further details about the design and construction of the habitat have been discussed in previous work.

Figure 1. (a) Recirculation diagram of the habitat; (b) Physical realization of the habitat.

The first and second compartments contain animals (consumers) and plants (producers), respectively. Snails are fed regularly with sinking algae tablets. The third compartment contains Bio-Fill, active carbon, and water filtration foam as the media serving the purpose of biological, chemical and mechanical filtration. The fourth compartment allows access for sensors and the water pump. The sensors used include dissolved oxygen (DO), pH and ORP. The water circulates through the four compartments. The first compartment has a motorized hatch of 10cm×10cm and an aerator that allow for reconfigurability, making the system open (volatile) or closed (non-volatile) if necessary; this mechanism is triggered as a fail-safe mechanism when the DO levels reach a minimum of 2.0 [mg/L]. The second compartment holds the LED-lamp and gives access to a dosifier pump that provides a sodium bicarbonate solution to increase the carbonate hardness (kH) of the water; the changes in kH are monitored through variations of the pH readings. Measurements from the sensors are processed by a computer/controller operating under LabVIEW®. The controller delivers the control signals that regulate the LED-lamp power via a pulse-width modulation (PWM) board, and also controls the hatch, and the air and dosifier pumps. The control signals can be generated by control laws or driven manually through a graphical user interface (GUI).

C. Organization

The paper is divided in five additional Sections. Section II presents the physico-chemical model while Section III introduces ecophysiological phenomena to the description of the aquatic habitat. Section IV presents the simulations performed and the results obtained, and Section V elaborates on discussions. Finally, Section VI provides concluding remarks and suggests research directions.
II. Physico-Chemical Model of the Aquatic Habitat

The physico-chemical description of the aquatic habitat makes use of a control volume for each compartment. The assumptions made in the formulation of the general mathematical model are as follows: (a) recirculation flow is assumed laminar; (b) water density is constant; (c) the recirculation flow is the same for all compartments; (d) liquid solutions are perfectly well-mixed in all compartments; (e) output concentrations are those inside each compartment; (f) the water level of all compartments is the same and constant; (g) the volume of the compartments is constant.

A. Mass Balance in Recirculating Systems

For a substance \( x \) the mass balance equation is written as:

\[
V \dot{x}_i = F_{in}[x]_{in} - F_{out}[x]_{out}
\]

where \( V \) is the control volume defined for the mass balance, \([x]_i\) is the concentration of the substance \( x \) inside the control volume in milligrams per liter [mg/L] or parts per million [ppm], \( F_{in} \) and \( F_{out} \) are the incoming and outgoing flow rates in [L/h], and \([x]_{in} \) and \([x]_{out} \) are the concentrations of those flows, respectively. The rate of change of the concentration \([x]_i \) multiplied by the control volume \( V \) defines the rate of accumulation of \( x \) in [mg/h]. For a recirculating system, the incoming and outgoing flow rates are the same. If the flow-rate is time dependent, the model is a non-linear system. Therefore, for a recirculating system with \( n \) compartments and a variable flow \( F(t) > 0 \) the general mass balance is expressed as:

\[
A_i \dot{x}_i = F(t) ([x]_j - [x]_i); \quad \forall \{1 \leq i \leq n \} \in \mathbb{R}; \quad j = \left\{ \begin{array}{ll}
 n & i = 1 \\
 i - 1 & \forall i \neq 1
\end{array} \right.
\]

(1)

where \( A_i \) is the surface area of each compartment and \( h \) is the height of the water level for all compartments.

B. Diffusion at Reduced Recirculation Flow Rates

Diffusion becomes dominant when \( F \approx 0 \) and a description for the gradient concentration between adjacent compartments becomes necessary. With Fick’s law of diffusion, the transfer between the two compartments is proportional to the following factors: (1) the concentration difference between them, (2) the equivalent cross-sectional area \( A_s \) through the separators, and (3) a constant \( D \). The complete general equation for a closed recirculating system of \( n \) compartments with \([x]_i \leq [x]_i \leq [x]_k \) is:

\[
A_i \dot{x}_i = f_{r.i} = F(t) ([x]_j - [x]_i) + DA_{s_{k,i}} ([x]_k - [x]_i) + DA_{s_{i,i}} ([x]_i - [x]_i)
\]

(2)

\[
k = \begin{cases}
 i + 1 & i \neq n \\
 i & i = n
\end{cases}; \quad l = \begin{cases}
 i & i = 1 \\
 i - 1 & i \neq 1
\end{cases}
\]

Parameters \( A_{s_{k,i}} \) and \( A_{s_{i,i}} \) are the equivalent cross-sectional areas between the compartment \( i \) and the adjacent compartments \( k \) and \( l \), respectively. Note that, with the definitions of \( k \) and \( l \), one of the diffusion terms is zero for the first and last compartments given that they only have one adjacent compartment.

C. Reconfiguration into an Open System

The model can be reconfigured into an open (volatile) system by allowing the transfer of gases between the water and the atmosphere. The expression used to model the mass transfer (i.e. oxygen and carbon dioxide) between the water and the atmosphere is based on Henry’s law of gas solubility and Fick’s first law of diffusion. The transfer is proportional to the contact surface area \( A_i \) between gas and liquid phases, the concentration difference between the liquid phase \([x]_i \) and the equivalent concentration of the gas phase \([x]_{atm} \), and a constant \( k_v \). The equation for a reconfigurable recirculating system is:

\[
\dot{x}_i = \frac{1}{h} \left( f_{r.i} A_i + k_{v,i} ([x]_{atm} - [x]_i) u_\sigma \right); \quad \forall \{1 \leq i \leq n \} \in \mathbb{R}; \quad u_\sigma = \begin{cases}
 0 & \text{non-volatile} \\
 1 & \text{volatile}
\end{cases}
\]

(3)

where \( u_\sigma \) is a switching signal that activates only one of the configurations at a time.
III. Biological Processes and Models of Ecophysiological Phenomena

Biological processes affect Equation 3 by adding a term $x_i$ to $f_{r,i}$ to account for the rate of production or consumption of the substance $x$ in the compartment $i$ in [mg/h].

$$[x]_i = \frac{1}{h} \left( \frac{1}{A_i} (f_{r,i} + x_i) + k_{v,i}([x]_{atm} - [x]_i) u_σ \right)$$ (4)

Such rates represent a measure of how chemical substances are produced or consumed in a given compartment. This paper makes use of this term in Equation 4 to introduce ecophysiological phenomena in the mathematical description of the aquatic habitat. In particular, this term is used to describe (1) animal and (2) botanical elements. Snails are modeled through their rate of consumption, treated as a random variable to account for changes in metabolic rates and aestivation. Aestivation consists in brief periods of torpor of the metabolism of the snails (similar to hibernation) in which oxygen consumption is considerably reduced. The plants, instead, are modeled through their rate of CO$_2$ assimilation as a function of irradiance. The following Subsections present these two models. Because this research focuses on respiration, the life support compounds considered are dissolved oxygen (DO), carbon dioxide (CD), carbonate hardness ($kH$).

A. Animal Component: Population of Pomacea Snails

The rate of O$_2$ consumption, DO, and CO$_2$ production, CD, by the respiration of a population of snails are modeled by differential equations with time constant $\tau$ and a random number of Gaussian distribution with mean $\mu \geq 0$, variance $\sigma^2$, and sample time $T$:

$$\frac{d}{dt} DO(t) = -\frac{1}{\tau} \left[ DO(t) + rand(\mu, \sigma^2, T) \right]$$ (5)

$$\frac{d}{dt} CD(t) = \frac{1}{\tau} \left[ CD(t) + rand(\mu, \sigma^2, T) \right]$$ (6)

The models in Eqs. 5 and 6 are proposed from observations in the validation of the temporal response of the model with Blum-type experiments, to be presented in Section IV.

B. Botanical Component: Rate of CO$_2$ Assimilation in Bacopa Monnieri

Photosynthesis is proportional to irradiant energy up to a limit in which plants reach their capacity to assimilate carbon dioxide. This phenomena is due to light saturation in chloroplasts as described by the light-response curve of Figure 2 and approximated by Equation 7 as a non-rectangular hyperbola. In Equation 7, $A$ represents the assimilation rate in [$\mu$mol/m$^2$/s], $I$ is the irradiance in [$\mu$mol/m$^2$/s], $\phi$ is the slope or the light-limited region, $\Theta$ determines the point of saturation by carboxylation, $A_{max}$ is the upper boundary of assimilation, and $R_d$ is the dark respiration of the plant. The light compensation point (LCP) in Figure 2 represents the irradiance value in which photosynthesis and dark respiration have equal magnitudes and result in a zero net assimilation of CO$_2$.

$$A = \frac{\phi \cdot I + A_{max} - \sqrt{(\phi \cdot I + A_{max})^2 - 4 \cdot \Theta \cdot \phi \cdot I \cdot A_{max}}}{2 \cdot \Theta} - R_d$$ (7)

![Figure 2. Light-response curve of photosynthesis to irradiance.](image)
IV. Simulations and Results

A. Simulations

The simulations prepared for this paper are based on the model and parameters presented in previous work for an aquatic habitat of 10 gallons and four compartments,\textsuperscript{14,19} with the addition of the biological models presented in Section III of this paper. Three simulations are presented: (1) the validation of the model with a Blüm-type experiment,\textsuperscript{5} (2) introduction of a model for the animal component to approximate results from the validation, and (3) the addition of the model of botanical elements to compare system performance under three light-response curves. The following Subsections provide additional details of each simulation.

1. Validation with a Blüm-type Experiment

The rates of consumption and production used for this particular paper are shown in Table 1. These parameters serve to approximate the performance of the simulations to the response obtained from a 7-day experiment in installed hardware. Subscripts in $DO$, $CD$, and $kH$ denote their associated compartment. The variable $[DO]_4$ represents the concentration of dissolved oxygen in the fourth compartment, which in this system is regulated through photosynthesis between 6 and 7 [mg/L] with an on/off controller driving the LED lamp. The simulations are implemented with a stiff Mod. Rosenbrock numeric method with maximum step of 0.01, with initial conditions $[DO] = 6.106$ [mg/L], $[CD] = 6$ [mg/L], and $[kH] = 95$ [mg/L].

\begin{table}[h]
\centering
\begin{tabular}{cccccccc}
\hline
 & $DO_1$ & $CD_1$ & $DO_2$ & $CD_2$ & $DO_3$ & $CD_3$ & $kH_3$ \\
Values & -4 & 4 & 23.0 & -23.0 & -7.0 & 7.0 & -17 \\
\hline
\end{tabular}
\caption{Production and consumption rates in [mg/h]}
\end{table}

2. Simulation of Consumer Model

As mentioned in Section IIIA, models in Equations 5 and 6 are proposed from observations in the Blüm-type Experiment. The simulation compares the steepness of the DO signal in the Blüm-type validation for a consumer/produce model with parameters $1/\tau = 5$ [rad/s], $\sigma^2 = 10$ [mg/h], and $T = 1$ [h]. The mean value $\mu$ of the Gaussian distribution are $DO_1$ and $CD_1$ from Table 1. These parameters were obtained by testing and comparing various other values, which were not included in Section IVB2 for clarity.

\begin{align}
DO_1 &= -\frac{1}{s + 1/\tau} rand(\mu, \sigma^2, T) \\
CD_1 &= \frac{1}{s + 1/\tau} rand(\mu, \sigma^2, T)
\end{align}

3. Simulation of Botanical Elements

Equation 7 approximates the mole to mole relationship of CO$_2$ assimilation in higher plants as a function of irradiance. Such relationship is adapted here to address the consumption of CO$_2$ as a function of the percent lamp power, $P_1[\%]$. As such, $A_{max}$ is replaced by $CD_{max}$ to account for the upper bound of CO$_2$ consumption. Equation 10 presents the modified light-response relationship and Figure 3 shows three curves for different values of $\phi$. Additional parameters are $CD_{max} = 23$ and $\Theta = 0.95$. All other parameters are similar to Section IIIB. This paper does not consider the dark cycle of respiration in the plants, i.e. $Rd = 0$.

\begin{align}
CD_2 &= -DO_1 = \frac{\phi \cdot P_1[\%] + CD_{max} - \sqrt{(\phi \cdot P_1[\%] + CD_{max})^2 - 4 \cdot \Theta \cdot \phi \cdot P_1[\%] \cdot CD_{max}}}{2 \cdot \Theta} - Rd
\end{align}

This simulation makes use of a proportional-integral (PI) controller that regulates the DO concentration in the fourth compartment, with a reference signal with a duty cycle of 18 hours for every 24. Such duty cycle helps to account for the physiological requirements of the botanical elements. The PI controller uses $P = 200$ and $I = 50$. The reference alternates between 6.75 and 6.25 [mg/L].
B. Results

1. Blüm-type Validation

Figures 4 and 5 show the validation of the mathematical model\textsuperscript{14,19} of the aquatic habitat for the parameters presented in Table 1. Signals in color are from the hardware, while black ones are from simulations. Figure 4 shows the DO and pH values, while Figure 5 shows the “steepness”\textsuperscript{5} of the DO signal, i.e. its derivative.

2. Consumer Model

Given the changes in rates of consumption of O\textsubscript{2} and production of CO\textsubscript{2} by the snails, Figure 6 compares the first two days of data. The intention is to have a measure of the variance of the steepness in DO, allowing the model to account for metabolic variations in the animal component of the system (consumers).
3. Botanical Model

Figure 7 presents the temporal response of the habitat, including DO, pH, and lamp power signals for \( \phi = \{0.3, 0.6, 1.5\} \). The main observation in this case refers to the similarity in DO and pH responses versus the different behaviors obtained for the lamp power signal.

![Figure 7. Comparison of three light-responses in simulations including animal component.](image)

V. Discussion

Results from the Blümm-type simulation validate the model of the aquatic habitat and the design proposed in previous work.\(^{14}\) Especially, the combination of measurements from hardware and validation of the simulation enable forensic analyses of the system to obtain the initial value of carbonate hardness, at 95 [mg/L], and its rate of consumption, at 17 [mg/h]. Figure 4 highlights the comparison between the DO and pH signals, for simulation and hardware. Although there are periods of time, up to days, in which the signals overlap well, there are others that show lack of synchronism. This is due to the on/off control used (like a thermostat) and the disturbances introduced by the population of snails (consumers). Until this validation, it was not expected that the behavior of snails would considerably disturb the time response of life support variables, i.e. these were assumed to be approximately constant and without disturbances. However, the Blümm-type validation allowed the discovery of the aestivation or metabolic depression\(^2\) that snails may undergo. This is particularly evident in Figure 5, which shows the rates of accumulation and depletion of oxygen in the habitat. While for a balanced system the steepness of the simulation respectively predicts a square signal between -0.2 and 0.2 [mg/L/h] of depletion and accumulation, the response obtained from hardware shows apparently random variations around those same values. This is why Section IVA2 proposes Equations 5 and 6 as the models for the animal component of the system, which is compared with the steepness signal of the validation in Figure 6. The result of using a random variable with a first order filter seems to be a fair first approximation to the behavior and disturbances introduced by the consumers. These simulations have to be limited to two days, because the disturbances trigger the on/off control at different times and encourages loss of synchronism, and further distorts the ability to compare the signals. However, the intention of such comparison is to achieve an approximate value for the variance \( \sigma^2 \), \( 1/\tau \), and \( T \) which in this case have been set in 10 [mg/h], 5 [rad/h], and 1 [h], respectively. The meaning of these values is: the rate of consumption is 4 [mg/h], but may change randomly every \( T = 1 \) [h] with a dispersion \( \sigma^2 = 10 \) [mg/h] and a time constant \( \tau = 0.2 \) [h]. In contrast to the on/off control used in the second simulation, Figure 7 makes use of setpoint control and photoregulation, and studies three light-response curves and their effects on simulations. Even though these simulations make use of the disturbances proposed for the consumer model, very small differences are noticeable in the time response of life support variables, DO and pH. This is especially true in the temporal response of pH, for which the three signals overlap. Another observation is found in the time response of the lamp power: the robustness apparent in the temporal response of the life support signals for a PI controller is product of the changes that occur in the lamp power signal. These show periodic steady-state values between 10 and 40 [%], for different values of \( \phi \). This distribution is expected from Figure 3. The curve with smaller \( \phi \) will require more lamp power to achieve similar values of CO\(_2\) assimilation.
VI. Conclusion

This paper elaborated on the model of an aquatic habitat for experiments relevant to closed-loop LSS and BLSS. It presented ground-based aquatic habitats as an option for small-scale BLSS research focusing in the process of respiration, and expanded the description of biological processes by introducing models of ecophysiological phenomena for consumers and producers. The model of the plants includes a description of the rate of CO$_2$ assimilation as a function of irradiance. The snails instead are modeled through their the rate of consumption, treated as a combination of a constant and a random variable to account for changes in metabolic rates and aestivation. Simulations and validation runs with hardware show how these phenomena may act as disturbances and introduce non-linearities. Other applications of the aquatic habitat as a small-scale experimental capacity may in the future include time-varying parameters in the botanical model to account for their growth, and to enable exploration of robust-adaptive approaches to their control.

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