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RESEARCH ARTICLE

HYBRID MODELING PREY PREDATOR-GENETIC ALGORITHM OF MOLD GROWTH DURING CACAO BEANS STORAGE

Diomande Siaho¹, Pandry Ghislain¹, Kadjo Tanon Lambert¹, Kakou Kouassi Ernest², Oumtanaga Souleymane¹ and Assidjo Nougou Emmanuel²

1. Laboratoire de recherche en Informatique et Télécommunication(LARIT), Institution polytechnique Félix Houphouët-Boigny (INP-HB), Yamousoukro, Côte d'Ivoire.
2. Laboratoire des Procédés Industriels de Synthèse et Environnement(LAPISENS), Institution polytechnique Félix Houphouët-Boigny (INP-HB), Yamousoukro, Côte d'Ivoire.

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Abstract

The production and quality of cocoa beans remain key issues for the economy of Côte d'Ivoire. The fairly humid Ivorian climate promotes increased mold production, leading therefore to a considerable negative impact on beans quality. In this work, a prey predator model was proposed to simulate the molds growth on cocoa beans. Our model (MPM), based on that of Leslie Gower, was identified using a multi-objective genetic algorithm (MOGA). The developed model allows to stimulate the relationship between parameters (i.e. sugar content (Su) and molds (M) with a good accuracy (R=0.9963 and 0.8382 respectively for molds growth and sugar content).

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Introduction:-

The stored grain ecosystem is made of interactions between its physico-chemical parameters, surrounding environment and pests (i.e. molds, insects, mites)(FLEURAT-LESSARD, 2017). Molds, microscopic fungi are at the origin of degradation of any organic matter on which they profit. Their presence increases challenges to store seeds because of toxins they produce(KEDJEBO, 2016; SARA & GHANIA, 2019). Thus, molds presence and proliferation are due to humidity and heat that emanate from biological activities in grains in general and cocoa beans in particular.

This study focuses on cocoa beans because of their essential role in the economy of several countries including Côte d'Ivoire. The quality loss impacts negatively the economy and performance of cocoa industries face to the international standards (ISO 34101, s. d.). Mold elimination in cocoa beans storage chain is currently debating in the scientific community (Barel, s. d., 1985; Cruz et al., 2020). Many methods have been proposed to eliminate them (e.g. storage environment atmosphere control (atmosphere composed of inert gases), hermetic storage, vacuum storage)(Barel, s. d., 1985; Cruz et al., 2020). Consequently, molds can lead to deterioration of their initial quality (Cruz et al., 2020). Therefore, cocoa beans storage is very challenging because of hot and humid climate in Côte d'Ivoire. Molds are one of the main causes of long-term storage loss (Cruz et al., 2016).

They also constitute a public health problem because of mycotoxins they can produce. Faced to this problem, some authors have opted for traditional methods, such as permanent control of cocoa beans physico-chemical parameters (temperature and moisture content, etc.), control of cocoa beans storage environment atmosphere...(Barel, s. d., 1985; Cruz et al., 2020; Ernest et al., 2015). However, these methods remain expensive and difficult to implement.

Corresponding Author:- Diomande Siaho

Address:-Laboratoire de recherche en Informatique et Télécommunication (LARIT), Institution polytechnique Félix Houphouët-Boigny (INP-HB), Yamousoukro, Côte d'Ivoire.

So mathematical approaches relating to molds growing on various supports (substrates) are proposed (E & F, 2002; Hukka & Viitanen, 1999; Kaleta & Górnicki, 2013). It is important to note that there are very few mathematical approaches modelling mold evolution in cocoa beans. Although, the literature about mold points out some typical models for some materials (Hukka & Viitanen, 1999; Ndiaye et al., 2002; Vereecken et al., 2015), and cereals (E & F, 2002; Kaleta & Górnicki, 2013). These so-called qualitative models set a critical threshold that depends on temperature and / or relative humidity above which a proven risk exists (Berger et al., 2018). For example, Jacobsen et al (E & F, 2002) proposed a linear model which takes account grain moisture (A_w) and temperature (T) as input parameters, in order to predict time elapsed before molds appearance during storage. Based on these same parameters, Ndiaye et al (Ndiaye et al., 2002) proposed a preventive approach (i.e. QualiGrain) of maximum storage time. Indeed, these models enable to predict the grains shelf life. However, they are static because they do not take into account the phenomenon temporal aspect. In addition, they are, a priori, based on predefined schedules with corrective interventions which are applied after damage observed (Fleurat-Lessard, 2017). To overcome these limits, several authors have turned to dynamic models defined by ordinary differential equations (ODE) (Berger et al., 2018; Hukka & Viitanen, 1999; Vereecken et al., 2015). For this purpose, approaches have been proposed in literature to predict risks of mold contamination as a function of relative humidity and temperature conditions (Barel, 1985). Among them, the VTT model has been proposed for wood and other building materials (Hukka & Viitanen, 1999). This model is one of the first in the construction industry, and has intensively been used. However, according to studies carried out by Berger et al (Berger et al., 2018), VTT model presents some limits because the determined parameters (e.g. k_{11} , k_{12}) are not included in the range of classes defined by this model. This work showed that mathematical formulation of mold growth VTT physical model is unreliable. Furthermore, these results showed that a small numerical value modification (about 1%) of VTT model parameter generates a prediction error of 94%. They therefore proposed a logistics model to improve the VTT one. However, even this last model (Berger et al) does not take into account mold growth variation under different humidity and temperature conditions. Most of these models focus only on mold population without considering the potential interactions that may exist in substrate environment in which they grow. In fact, mold evolution is strongly correlated to the substrates physicochemical parameters one, leading therefore to the proposition of a prey predator type differential equation model. This model considers each individual in a population and simulate its behavior and interaction with other individuals (Luckinbill, 1973). Prey-predator models enable to explain and provide solutions to the complexity of various ecosystem (Camara, s. d.). The first models were proposed by Lotka and Volterra in the 1920s, to explain the oscillatory phenomenon with phase shift of prey and predators abundance (Abid, 2016). These models have drawn considerable attention in applied mathematics and theoretical ecology. However, in (Abid, 2016) criticisms are made about the linear relationship between attack rates and predator size. Therefore, Leslie and Gower proposed a predation model improvement by integrating, as an hypothesis, a limit threshold representing resources maximum capacity for prey and predators (Leslie & Gower, 1960). Thus, this basic hypothesis (Du et al., 2019) confers to it the class of a realistic model and was therefore used for several areas (e.g. health, biological control, fisheries to regulate excessive fishing). These models (prey predator type) are still untapped for prediction of mold evolution in cocoa beans. Among all these models, Leslie-Gower one is suitable to investigate the case of interactions between cocoa beans and molds.

Unfortunately, in the case of cocoa beans storage, very few studies concerning modeling of mold growth were carried out. The purpose of this present study is to propose a growth model of molds evolution via the predator-prey model (Leslie Gower).

Materials and methods:-

In the purpose of modelling molds growth on cocoa beans during their storage, the Leslie-Gower model was used combined to a multi-objective genetic algorithm (MOGA). Indeed, the latter was used for Leslie Gower specific parameters identification.

Leslie Gower Model:

In our approach, we considered Leslie Gower (Eq. 1) prey predator model as the one that simultaneously obtains the prey and predators density over time by taking into account the available resource relative to each population. In this model, the predation term can be written in different ways depending on the response functional type. There are three types according to the problem to be solved (Abid, 2016). On this subject, in (Luo et al., 2020) the authors state that the functional response is a determining element of predation. Thus, whether it is linear (Holling type I), nonlinear (Holling type II) or sigmoid (Holling type III), it helps to better understand the relationship between prey and predator. In the case of our study, we opted for the Holling type I functional response which results in (Abid,

2016). And this means that the variation in predation evolves proportionally to encounter rate between predator and prey. This model looks like this:

$$\begin{cases} \frac{\partial U}{\partial t} = \mu U \left(1 - \frac{U}{V}\right) - \lambda UV \\ \frac{\partial V}{\partial t} = \rho V \left(1 - \frac{V}{\theta U}\right) \end{cases} \quad (1)$$

Where $U(t)$ represents prey population and $V(t)$ the predator one at time t .

$\mu \geq 0$, $\lambda \geq 0$, $\rho \geq 0$ and $\theta > 0$ are parameters representing the interaction between these two species. μ denotes the prey population growth rate in the absence of predator. λ represents predator attack rate, θ represents the conversion efficiency (percentage of consumed biomass that is converted into predator biomass), ρ the predator mortality rate

and μ the growth rate of the prey population in the absence of predator. $\frac{U}{\theta V}$ is called the Leslie-Gower term and measures the loss of prey density (Abid, 2016).

The approach proposed in this work aims to predict the behavior of molds over time by considering sugar content dynamics. For Berger et al. (Berger et al., 2018), the model robustness follows a good model parameters identification. This is based on the formulation of inverse problems (El Mankibi et al., 2019) consisting in minimizing a cost function that establishes the discrepancy between experimental data and modeling results one. As a result, several methods exist in literature such as gradient method (Fouka et al., 2017), genetic algorithm (Zaghdoud, 2020), Monte Carlo method (Fan et al., 2019)... However, the most representative methods are the genetic algorithm (GA) ones due to their ability to determine the optimal solution (s) knowing a part of the evolution of the system to be optimized (SAADALLAH, s. d.). Thus, in this contribution, genetic algorithms have been used to identify our model parameters.

Genetic Algorithm:

Genetic algorithms are stochastic optimization algorithms classified in the meta-heuristics family. These algorithms are based on the mechanism of natural selection and genetics (Darwin) (Djilali Beida, 2017). They have grown considerably because of their ability to not impose any conditions on the nature of the functions to be optimized. They enable to manipulate a set of solutions through several iterations to converge towards optimal solutions. Its operating principle and initial parameters are detailed in research work carried out in (Djatouti et al., 2019).

In our approach, 5 parameters were identified by optimizing the objective or fitness function that has been used to evaluate individuals in a well-defined research space. It is also necessary to assign data to the GA operators, namely selection, crossover and mutation. To accomplish this, each parameter to be identified must be encoded by a gene using either binary or real representation. In this present work, real representation was chosen to avoid difficulties that can be raised on the binary encoding and decoding of chromosome. It is important to note that AGs can operate with one or more objective functions. This last case concerns multi-objective optimization. This optimization uses the Pareto dominance notion to classify solutions and define selection strategies (reproduction or survival). They keep the best solutions in the population over generations or save them in an archive. From the compromises of objective functions, an equilibrium called Pareto optimum is reached. According to (Murugan et al., 2018) one solution dominates another if it is better with respect to all criteria. Based on this concept of dominance, the aim of the optimization algorithm is to determine the Pareto front, that is, the set of non-dominated solutions. For this purpose, the Pareto-based approaches used with success are VEGA (Vector Evaluated Genetic Algorithm) (Zhang et al., 2020), MOGA (Multi Objective Genetic Algorithm) (Sada, 2020), NSGA (Non Dominated Sorting Genetic Algorithm) (Choi & Song, 2019), NSGA II (Pham et al., 2020), PAES (Pareto Archived Evolution Strategy) and SPEA (Strength Pareto Evolutionary Algorithm) (Yang-geng et al., 2019). These approaches have different strategies. Indeed, the difference lies in the distribution of the solutions on the front and in the convergence speed. The principle of MOGAs is more specific at the assessment stage preceding the selection one. Indeed, this step is subdivided into two operations, namely the solution quality assessment in terms of convergence and diversity.

A multi-objective optimization problem is as follows (Merджаoui et al., s. d.):

$$\begin{cases} \text{Minimize } F(x); F \in R; \text{ with } F(x) = [f_1(x), f_2(x)] \\ \text{Such as constraints} \\ h_j(x) \leq 0; \quad j = 1, \dots, m; \quad x \in S \subset R^n \\ \text{Be satisfied} \end{cases} \quad (2)$$

Proposed Approach:

Our approach to predict mold evolution encompasses the growth and predation of mold on cocoa beans surface sugars. This predation is illustrated in Fig. 1;

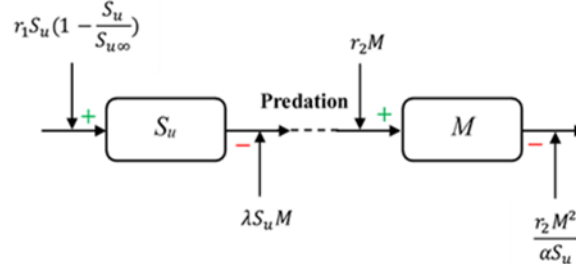


Figure 1:- Prey Predator diagram (molds - sugar).

Problem Formulation:

Leslie Gower model aims modelling prey predator interactions according to verhurst law. Thus, this technique use is justified in our case, because molds have an impact similar to that of a predator on cocoa beans. In fact, to feed themselves, molds proceed by absorption of surrounding organic matter (carbon source); hence their so-called heterotrophic way of life (« L’univers des champignons », 2018). To obtain the herein prey predator model, sugar content was indexed as prey and molds as the predator. According to literature, water content promotes molds development. However, sugars which coating the tegument, constitute one of the carbon sources and therefore food for molds. Thus, Leslie Gower model enables to determine molds evolution according to sugar amount observed regularly. In our work we assume that:

- (i) mold development depends mainly on sugar coated on beans;
- (ii) all beans have the same sugar content after drying.

Mathematical Model:

Using the Leslie Gower model as defined previously (section 3), it is necessary to determine molds amount as well as sugar content over time. Then formulation (1) after correspondence of the different terms, becomes formula (3). All paragraphs must be indented.

Let’s denote by $S_u(t)$ the sugar content and $M(t)$ the mold (biomass) rate at time t (weeks) .With:

- $S_{u\infty}$: The sugar maximum content on beans
- r_1 : The growth rate of sugar content
- λ : The contamination rate of beans by molds
- r_2 : The mold growth rate
- M_∞ : Mold maximum capacity
- α : the sugar content conversion into mold (constant).

Mold and sugar evolutions are represented by the following pair of differential equations called herein MPM (Mold Predictive Model):

$$\begin{cases} \frac{\partial S_u}{\partial t} = +r_1 \cdot S_u \cdot \left(1 - \frac{S_u}{S_{u\infty}}\right) - \lambda S_u M \\ \frac{\partial M}{\partial t} = r_2 \cdot M \cdot \left(1 - \frac{M}{M_\infty}\right) \quad \text{with } M_\infty = \alpha T_e \end{cases} \quad (3)$$

Identification Process:

The objective functions optimization leads to the identification of parameters vector $y^T = [r_1 S_{u\infty} \lambda r_2 \alpha]$, shown schematically in table 1.

Table 1:- Representation of a chromosome.

r_1	$S_{u\infty}$	λ	r_2	α
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This parameters identification is operated using the MOGA algorithm (Locteau et al., 2006).

Multi-objective Function:

In this section, the optimized bi-objective function J_r ($r =$ molds and sugar) is defined. Indeed, J_r represents the sum of the squares of the differences between the observed sugar / mold values and those calculated by Eq.(1) or (2), as follows :

$$\begin{cases} \text{Minimize } J; J \in R; \text{ with } J_{r=1,2} = [J_1(x), J_2(x)] \\ J_{r=1,2} = \sum_{i=1}^n [y(t) - y_{ob}(t)]^2 \end{cases} \quad (4)$$

Then, a genetic algorithm is applied in order to find the parameters best values that minimize these functions concomitantly. The optimisation using of the genetic algorithm was repeated 100 times with the operators values defined in Table 2.

Table 2:- GA initial conditions.

Parameters and operators	
Population size	200
Elite count	0
crossover rate	50%
mutation rate	0.05
No. of generation	200
Crossover function	@crossovercattered
Mutation operator	@Mutatio uniform
Selection function	@selectionstochunif
Diagnostic information	
Fitness scaling function	@fitscalingrank
Number of variables	5
Parameters variation interval	0 – 15

Experimental work:

The experimental data were obtained by measurements of biomass (molds) and sugar amount on cocoa beans tegument stored in jute bags for 24 weeks. The different bags were placed on pallets (1 m x 70 cm), in a store at room temperature (20-36 ° C).

Each week, three bags were taken randomly considering beans heterogeneity. The parameter value at a given time is then the mean one.

Mold determination:

Total fungal population count was carried out by surface inoculation on PDA medium (Potato dextrose agar) with chloramphenicol. This is a method that allows uniform molds growth because of equal access to oxygen (Hocking,

1991). The total population estimate (N), expressed in log UFC.g-1, is calculated according to the ISO standard (ISO 7218 / A1) (NF EN ISO 7218/A1 - Octobre 2013, s. d.).

Sugar content determination:

Sugar content determination was carried out by using Dubois sulfuric phenol method(Bourelly, 1980).

Results and Discussion:-

The different simulations were carried out using Matlab R2013a. The computer used characteristics were: 64-bitoperating system computer, 8 GB of RAM, Processor Intel Core i7.

The parameters $r_1, S_{u\infty}, \lambda, r_2, \alpha$ of the approach presented in section 4 were determined by minimizing the multi-objective function J_r using experimental data. The results of these simulations are presented by Fig.2, representing the Pareto front. It appears that the values of J_{sugar} are lower when $J_{biomass}$ ones are higher. However, the best value of J_r function two components is shown in red in this figure. It coordinates are (0.083; 0.547) and represents the best compromise between $J_{biomass}$ and J_{sugar} .

This minimum value corresponds to the individual presented in Table 1.

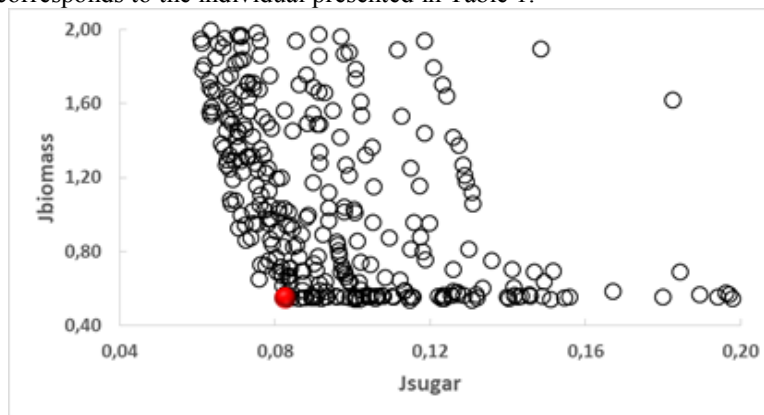


Figure 2:- The Pareto front.

Table3:-Identified parameters of the Leslie Gower model

Parameter	r_1	$S_{u\infty}$	λ	r_2	α
Value	13.055	1.345	0.608	0.348	3.865

These values, integrated into the differential equations system (2) and solved by the fourth order Runge Kutta algorithm, give the results presented in Figs. 3 and 4 for both calculated and experimental data respectively for biomass and sugar content.

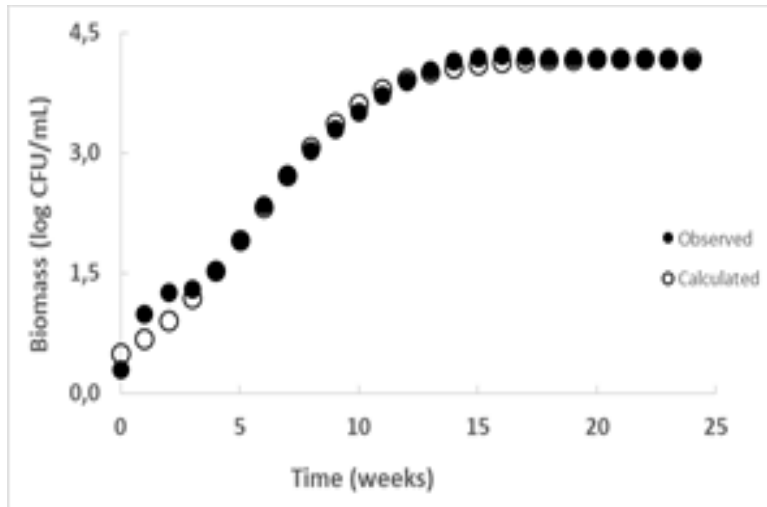


Figure 3:- Experimental and simulated curve of the evolution of molds.

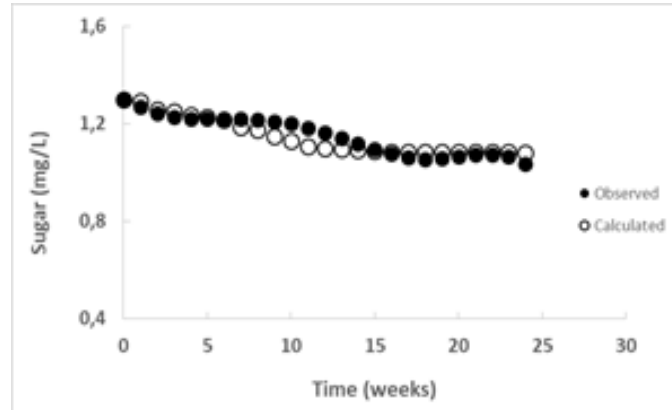


Figure 4:- Experimental and simulated curve of the evolution of the sugar content.

The analysis of Fig. 3, shows that the biomass increases gradually from week 0 (0.30 log CFU / g) to week 15 (4.11 log CFU / g). Then it stabilizes until the end of the experiment (24 weeks). On the other hand, the sugar content decreases steadily until week 15 to stabilize (Fig 4).

Furthermore, it is clear from the two figures that the calculated values fit correctly the experimental ones with a correlation coefficient $R = 0.9963$ and $R = 0.8382$, respectively for the biomass and the sugar content. This result shows a good accuracy of Leslie Gower model for modeling mold growth on cocoa beans during 24 weeks storage. These observations are in agreement with those reported in Ref. 16 for molds on different supports.

However, there is a slight discrepancy between experimental and observed data in particular, with regard to the sugar content, between the 7th and 16th weeks. This fact could be due to phenomena (impact of relative humidity, temperature ...) not considered in our model.

Conclusion:-

In this paper, a mathematical model of mold evolution in cocoa beans based on prey predator models of the Leslie Gower type was proposed. A multi-objective genetic algorithm was also used for its parameters identification. The results obtained show a good accuracy between experimental and the proposed model calculated values, indicating that Leslie Gower models are suitable for modeling molds growth during cocoa beans storage.

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