Applying Membrane Systems in Food Engineering

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Summary. Food engineering deals with manufacturing, packaging and distributing systems for drug and food products. In this work, we discuss about the applicability of membrane systems to model environmental conditions and their effects on the produces during storage of fresh fruits and vegetables. In particular, we are interested in abstract molecular interactions that occur between produce, film and surrounding atmosphere factors involved in fresh fruit and vegetable package designs. We present a basic implementation to simulate the dynamical behaviour of these systems, due to gas exchanges and temperature fluctuations. Additionally, we reveal the benefits of this modelling approach and suggest some extensions as future directions to be considered.

1 Introduction

Membrane systems [17], also called P systems, had emerged to assist in the modelling of systems of concurrent reactions taking place in compartments, so as occur in biological systems. In this paper we use P systems as membrane structures delimiting compartments that contain multisets of objects representing molecules. The model was first presented in [3]. Compartments configuration changes over time (evolves) according to given rules that represent biochemical reactions and diffusions. In contrast to ODE-based approaches, each single molecule within the entire system is represented explicitly as individual entity. Capturing aspects of structural dynamics (changes in the membrane structure as well as in the composition of complex molecules) is seen as an advantageous feature of P systems. Inclusion of reaction kinetics into this formalism can be done by discretised kinetic laws [10]. We applied this mathematical formalism to a real known problem in fruits and vegetables post-harvest processing.

Fresh fruits and vegetables are living materials that continue to respire after harvesting exhibiting progressive biochemical changes. Food engineering methods to preserve freshness of post-harvest produces include low temperature storage and special packaging technologies, mainly Modified Atmosphere Packaging (MAP). MAP of fresh fruits and vegetables refers to the technique of enveloping the produce in a sealed container of polymeric film in order to modify the O_2 and CO_2 concentrations inside the package, reducing metabolic activity and increasing shelf life [16].

Designing MAP systems is a complex task that involves considerations about many interrelated environmental (as temperature and atmosphere composition), biological and package technology factors. Basic biological processes are respiration, transpiration, ethylene production and compositional changes due to metabolism. The variability of responses to internal and external signals depends on the characteristic of each plant organ type, developmental stage and physiological condition. In addition, much of the behaviour of a MAP system at cellular level are not fully understood. As examples we can refer to the little knowledge about the effect of CO_2 on the activity of respiratory enzymes [11]. Moreover, the contribution of the biochemical changes that alters physical properties of cell walls and tissues modifying the texture of the produce is not known in detail [9]. On the other hand, the mechanism of ethylene signal transduction that coordinates fruit ripening processes, is another aspect subject to study [1].

The difficulty to test different combination of gases and temperatures and the complexity of experimental setup for MAP systems had led to the development of various mathematical models [4, 11, 16, 19] and software [14]. In the literature, many respiration models are empirical fits of experimental data, based on one particular type and variety of fruit or vegetable, and most of them are based on the principles of enzyme kinetics and are represented using ODEs (for reviews see [5, 18]). However, there exists some lack on studies about the dynamical behaviour of these systems in terms of changes in environmental conditions, so as produce composition and physiology due to developmental processes [5]. It is worth mentioning that post-harvested fruits and vegetables, unlike other living materials, can be considered as less robust systems, as their responses on environmental fluctuations depends mostly on their actual configuration of biochemical components. In this context, some authors [7, 14] have considered the potential benefits of a systematic analysis or process-based modelling approach for fruits and vegetables. Considering that understanding the reaction network underlying MAP systems can give food experts more knowledge about emergent properties of packaged fruits and vegetables, we propose a framework based on membrane systems that abstracts basic biochemical reactions that occur in MAP systems. In the future, the proposed model can serve as a predictive tool to simulate changes in fresh produce on the molecular level, due to changes in environmental conditions.

This paper is organized as follows: firstly, biological and technical background of MAP systems is described in section 2. In Section 3 we present a P system framework for MAP, including the description of components, reaction kinetics

and evolution of the system. Section 4 shows an application of the framework considering a package under modified atmosphere containing two produces. Finally, in Section 5 we point out some benefits of using our framework and future extensions of it.

2 Fresh Fruits and Vegetables Packaging

From the horticultural point of view, there are four main, sometimes overlapped, developmental stages identified in fruits, vegetables and flowers: growth, maturation, ripening and senescence. For packaging technology purposes, maturation and ripening stages of fresh commodities constitutes the central point of attention. During ripening, fruits and vegetables suffer considerable physiological changes that normally include: modification of colour through the alteration of chlorophyll, carotenoid, and/or flavonoid accumulation; textural modification via alteration of cell turgor and cell wall structure and/or metabolism; modifications of sugars, acids, and volatile profiles that affect nutritional quality, flavour, and aroma; and, generally enhanced susceptibility to opportunistic pathogens (likely associated with loss of cell wall integrity) [8]. The climacteric is a stage of fruit ripening associated with an autocatalytic production of ethylene, that rises cell respiration in some fruits. This physiological process marks the end of fruit ripening and the beginning of fruit senescence, in which a serie of irreversible events leads to breakdown and death of the plant cells.

In addition to temperature control, a reduced O_2 and elevated CO_2 atmosphere can extend the post-harvest life of whole and pre-cut commodities. This techniques reduce their respiration rate as well as production of ethylene, minimizing metabolic activity, delaying enzymatic browning and retaining visual appearance [13]. In order to obtain a good design of such a system, it is necessary to understand many concurrent reactions at a macro, meso and micro level, including the dynamics behind the interdependencies between environmental, biological and technical factors.

Basic environmental factors to be consider in MAP design are temperature, relative humidity (RH), and atmosphere composition. Other minor factors are light, chemicals as fungicides, growth regulators, ethylene perception blockers, etc. Temperature is the most important extrinsic factor affecting all elements of harvested produce. Considering packaged produces, temperature influences both the gas exchange of the produce and the permeability of the film for O_2, CO_2 and H_2O.

High RH in the atmosphere surrounding fruit diminishes dehydration and preserves freshness, whereas excessive RH may engender moisture condensation, microbial growth and decay of the produce. On the other hand, three gases in the surrounding atmosphere O_2, CO_2 and ethylene (C_2H_4), mostly influence stored fresh fruits and vegetables. Decreasing oxygen partial pressure can increase shelf life, but it is essential that the oxygen level not be reduced to the point that anaerobic respiration occurs. Anaerobiosis results in fermentation, the chemical conversion of

carbohydrates into ethanol and organic acids, which may cause undesirable odours and flavours. Ethylene is a gaseous plant hormone (signal molecule) that regulates fruit ripening and senescence. O_2 is required for the synthesis of ethylene, while O_2 and low levels of CO_2 are required for its biological activity [9].

The most important biological processes occurring in fresh fruits and vegetables that affect them in packaging conditions over time are respiration, transpiration, ethylene production and compositional changes due to metabolism. Additionally, developmental processes, so as physiological and pathological breakdown should be considered.

Respiration involves a complex set of biochemical processes of which part is the oxidative breakdown of carbohydrates, lipids and organic acids into CO_2 and H_2O plus heat and metabolic energy. Respiration rate can be expressed in terms of O_2 consumed or CO_2 produced. The respiratory quotient (RQ), the ratio of CO_2 produced to O_2 consumed, ranges from about 0.7 to 1.4 depending on the substrate and its metabolic state (if the substrate is a lipid, $RQ < 1$, and $RQ > 1$ for organic acids)[5]. When carbohydrates are aerobically respired, the RQ is near 1, and the reaction is represented by Eq. (1).

$$C_6H_{12}O_6 + 6\,O_2 \rightarrow 6\,CO_2 + 6\,H_2O + energy \tag{1}$$

On the other hand, post-harvested fresh fruit and vegetables are mainly made up of water (80 to 95% approx.). Water loss is the primary cause of fresh weight loss and it is much more sensitive to changes in relative humidity around the commodity than to the rate of respiration[9]. Transpiration occurs due to the fact that fruits and vegetables internal atmosphere is saturated with water vapour, while external atmosphere contains lesser. Therefore, water loss rate depends on the external and internal water vapour pressure gradient.

There are two types of MAP techniques: passive or active. Passive MAP or equilibrium modified atmosphere consists in matching film permeation rates for O_2 and CO_2 with the respiration rate of the packaged produce. In some cases, it is likely that atmospheres within MAP will be actively established and adjusted, and this is realised creating a vacuum into the package and replacing the atmosphere with the desired gas mixture, and/or introducing gas absorbers/emmitters or other atmosphere-modifying elements into the package, so as using specialized films [18].

In a MAP design process, the type of material and its surface area and thickness are selected to obtain the desired equilibrium gas composition. Each film type has specific ranges of O_2 and CO_2 permeabilities, usually with the permeability of CO_2 being $3 - 5$ times that of O_2 [4]. Two strategies for creating film barriers exist: continuous and perforated films. Continuous film control movement of O_2 and CO_2 into or out of the package so that steady-state O_2 and CO_2 levels are achieved in the package, that is, they are used in the MAP design process assuming a constant respiratory rate of the produce. Perforated films with small holes are more suitable for produce having a high O_2 demand, and in this case the rate of gas exchange is a sum of gas permeation through the film and gas diffusion through the microperforations [9].

3 A P System-based MAP

We abstract a fruit or vegetable as a graph of cells or modules, like tissue P systems [15]. Each cell represents a compartment that contains species, and at a specific time, the contents of the compartment determines the cell configuration. This serves as a mechanism to differentiate one cell from other, given the possibility to create diverse tissue types, as occurs for example in fruits epicarp, mesocarp and endocarp tissues [7]. Additionally, as gas consumption-production occurs inside the cells, at the mitochondria level, and is stated that gas diffusion between cells depends on the geometry of the produce [11], differences in gas content in cells that conform a determinate region can adequately be represented. This is also in accordance to the idea that the ripening process usually starts in one region of a fruit and spreads to neighbouring regions, due to ethylene diffusion starting from promoter cells [1]. Produces into the package are represented as a population of membranes, giving the advantage that the model can deal with distinct fruits and vegetables within the same film, or the same produce in distinct developmental stages, varieties and/or presentations. Figure 1 shows as example, the schematic representation for such a system. In the next section we present the formal specification of our model.

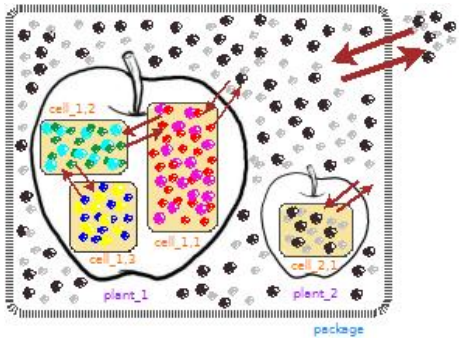

Fig. 1. A schematic representation for the MAP system model. In this case, two produces share a package: $plant_1$ is formed by three connected cells, and $plant_2$ is formed by a single cell. Arrows represent paths for molecules (spheres) diffusions

Multiset prerequisites

Let A be an arbitrary set and $\mathbb{N}$ the set of natural numbers including zero. A multiset over A is a mapping $F : A \longrightarrow \mathbb{N} \cup \{\infty\}$. $F(a)$, also denoted as $[a]_F$, specifies the multiplicity of $a \in A$ in F. Multisets can be written as an elementwise enumeration of the form $\{(a_1, F(a_1)), (a_2, F(a_2)), \ldots\}$ since $\forall (a, b_1), (a, b_2) \in F : b_1 = b_2$. The support $\text{supp}(F) \subseteq A$ of F is defined by $\text{supp}(F) = \{a \in A \mid F(a) > 0\}$. A multiset F over A is said to be empty iff $\forall a \in A : F(a) = 0$. The cardinality

$|F|$ of F over A is $|F| = \sum_{a \in A} F(a)$. Let F_1 and F_2 be multisets over A. F_1 is a subset of F_2, denoted as $F_1 \subseteq F_2$, iff $\forall a \in A : (F_1(a) \leq F_2(a))$. Multisets F_1 and F_2 are equal iff $F_1 \subseteq F_2 \wedge F_2 \subseteq F_1$. The intersection $F_1 \cap F_2 = \{(a, F(a)) \mid a \in A \wedge F(a) = \min(F_1(a), F_2(a))\}$, the multiset sum $F_1 \uplus F_2 = \{(a, F(a)) \mid a \in A \wedge F(a) = F_1(a) + F_2(a)\}$, and the multiset difference $F_1 \ominus F_2 = \{(a, F(a)) \mid a \in A \wedge F(a) = \max(F_1(a) - F_2(a), 0)\}$ form multiset operations. Multiplication of a multiset $F = \{(a, F(a)) \mid a \in A\}$ with a scalar c, denoted $\mathrm{c} \cdot F$, is defined by $\{(a, \mathrm{c} \cdot F(a)) \mid a \in A\}$.

P system components

Let $\mathbb{N}_+ = \mathbb{N} \setminus \{0\}$ be the set of natural numbers without zero, and $m, n \in \mathbb{N}_+$. We define a P system for a MAP system as a construct:

$$\Pi_{\mathrm{MAP}} = (\mu, S, plant_1, \ldots, plant_m, G, L_0, D_1, \ldots, D_d, f_1, \ldots, f_d, \Delta\tau)$$

where:

- $\mu = [[[]_{cell_{1,1}} \cdots []_{cell_{1,n_1}}]_{plant_1} \cdots [[]_{cell_{m,1}} \cdots []_{cell_{m,n_m}}]_{plant_m}]_{package}$ is the spatial system structure composed of three inner levels: package, plants, and cells,
- S is a set of chemical species,
- $plant_1, \ldots, plant_m$ represent the produces into the package,
- G is a set of global parameters,
- $L_0 : S \to \mathbb{N}$ is a multiset of axioms representing the initial molecular configuration,
- D_ν is a diffusion (communication) rule among package and external environment ($\nu = 1, \ldots, d$),
- $f_\nu : (S \to \mathbb{N}) \to \mathbb{N}$ is a kinetic function attached to diffusion rule D_ν,
- $\Delta\tau \in \mathbb{R}_+$ is the time discretisation interval.

A diffusion rule D_ν can be of the form $[s] \to []s$ for molecules $s \in S$ leaving the package and released to the external environment, and $[]s \to [s]$ for molecules entering the package, respectively.

Furthermore, each $plant_i$ is defined as a tuple:

$$plant_i = (N_i, E_i, G_i, D_{i,1}, \ldots, D_{i,d_i}, f_{i,1}, \ldots, f_{i,d_i})$$

where:

- $N_i = \{cell_{i,1}, \ldots, cell_{i,n_i}\}$ defines a set of cells within plant i,
- $E_i \subseteq N_i \times N_i$ specifies a set of directed edges (diffusion channels between cells),
- G_i is a set of plant (organ) specific parameters,
- $D_{i,\kappa}$ represents a diffusion rule inside plant i and between plant i and package ($\kappa = 1, \ldots, d_i$),
- $f_{i,\kappa}$ is a kinetic function attached to diffusion rule $D_{i,\kappa}$.

Here, a diffusion rule can be of the form $[s]_{cell_{p,q}} \rightarrow []_{cell_{p,q}} s$ for molecules $s \in S$ leaving $cell_{p,q}$ and spread out into the package. A rule of the form $[]_{cell_{p,q}} s \rightarrow [s]_{cell_{p,q}}$ describes molecules entering $cell_{p,q}$ from the package. Finally, a rule of the form $[s]_{cell_{p,q}} \rightarrow [s]_{cell_{x,y}}$ formulates the directed transport of molecule s along the edge $(cell_{p,q}, cell_{x,y}) \in E_i$.

Each $cell_{i,j}$ is defined as a tuple

$$cell_{i,j} = (L_{i,j,0}, R_{i,j,1}, \ldots, R_{i,j,r_{i,j}}, f_{i,j,1}, \ldots, f_{i,j,r_{i,j}})$$

where:

- $L_{i,j,0} : S \rightarrow \mathbb{N}$ is a multiset of axioms representing its initial molecular configuration,
- $R_{i,j,k} = (A_{i,j,k}, B_{i,j,k})$ with $A_{i,j,k} : S \rightarrow \mathbb{N}$ (multiset of reactants) and $B_{i,j,k} : S \rightarrow \mathbb{N}$ (multiset of products) specifies a reaction rule including its stoichiometric factors,
- $\mathrm{f}_{i,j,k} : (S \rightarrow \mathbb{N}) \rightarrow \mathbb{N}$ is a function corresponding to kinetics of reaction $R_{i,j,k}$.

System evolution

A P system of the form Π_{MAP} evolves by successive progression of its configuration at discrete points in time $t \in \mathbb{N}$ for what we assume a global clock. Two consecutive dates t and $t+1$ specify a time span $\Delta\tau$. A system step at time t consists of three modification stages carried out from outer to inner spatial components of the system. Firstly, the diffusion between package and its environment is considered. To this end, the rules D_1 up to D_d are employed. Afterwards, the diffusion between package and cells as well as the intracellular diffusion is utilised by employing the rules $D_{i,\kappa}$ for each plant $i = 1, \ldots, m$. The last modification stage concerns application of the reaction rules specified in each cell. To cope with conflicts that can occur if the available amount of substrate cannot satisfy all matching diffusion and reaction rules, we prioritise all rules by their index: $D_1 > D_2 > \ldots > D_d$. Moreover, for each plant i: $D_{i,1} > D_{i,2} > \ldots > D_{i,d_i}$ and for each cell i, j: $R_{i,j,1} > R_{i,j,2} > \ldots > R_{i,j,r_{i,j}}$. Thus, we keep determinism of the system evolution and enable mass conservation. An alternative method for coping with conflicts is randomisation in selection and sequentialisation of diffusion and reaction rules.

The application of an arbitrary rule is organised into two consecutive steps. The first step identifies all molecules from the rule's left hand side acting as sources for diffusion or reactants. These molecules are removed from the current configurations. Corresponding molecules from the right hand side (destinations in case of diffusion and products in case of reactions) are then added.

We formulate discretised reaction-diffusion kinetics by specification of scalar functions $f : M \rightarrow \mathbb{N}$ based on a multiset $M : S \rightarrow \mathbb{N}$. Each function f converts the current configuration (L_t or $L_{i,j,t}$), a multiset of objects, into the number of turns for application of the corresponding diffusion or reaction rule. Here, kinetic laws $\hat{\mathrm{f}}(s)$ for each species $s \in S$ employ the multiplicity of its occurrences to formulate the corresponding reaction rate.

For updating the entire system configuration, we define an iteration scheme as shown in Figure 2. When this formalism is hidden in a software, the specification is intuitive and accessible for an expert focussing on MAP modelling.

4 Simulation

As a first application, we introduced as rules into the model only the basic processes involved in a MAP design: respiration and fermentation, so as gas diffusion between membranes. The influence of gas composition on respiration rates of produce has been widely represented by Michaelis Menten-type equation [5]. In this context, respiration rate is considered as a function of concentration in terms of enzymatic reaction, with O_2 in the place of substrate and the product CO_2 acting as inhibitor.

Temperature dependence over respiratory rate and over film permeability was represented using Arrhenius equation (Eq. 2).

$$k = F \times e^{-E_a/R \times T} \tag{2}$$

where E_a is the activation energy, expressed in joule per mol, defined as the energy that must be overcome for a chemical reaction to occur; R is the gas constant ($\approx 8.314\ \ J \cdot K^{-1} mol^{-1}$), T the absolute temperature, F is the pre-exponential factor that represents the total number of molecular collisions per second; and k corresponds to the number of collisions per second that result in a reaction. This can be related to the probabilistic approach to P systems introduced by [2] in order to obtain more biological-like models. In this context, the Arrhenius exponential term can be viewed as the probability per time unit that the reaction takes place.

In order to apply our model, we simulate the dynamical behaviour of an instance of a Π_{MAP} with two hypothetical fruits as it is shown in Fig. 1, using continuous film and passive MAP as package techniques. Rules that use symbol $\rightleftharpoons$ between reactants and products must been interpreted as reversible reactions. Into the formalism described in Fig. 2, a rule of the form $D_\alpha = [\sigma] \rightleftharpoons []\sigma$, for example, consists in the following two rules, in order of application: $[\sigma] \rightarrow []\sigma$ and $[]\sigma \rightarrow [\sigma]$.

Temperature is represented by T and expressed in Kelvin (K). O_2, CO_2 and H_2O abundances in the outside are represented by $O2ex$, $CO2ex$ and $H2Oex$ respectively. A and E symbolise the surface area in cm^2 and the thickness of the packaging film in mil ($1mil = 0.00254cm$). $pO2$ and $pCO2$ represent the reference film permeability in $mL \cdot mil \cdot cm^2 \cdot hr^{-1} \cdot atm^{-1}$ for O_2, CO_2 and H_2O, respectively. $EaO2$ and $EaCO2$ symbolise the permeability activation energy expressed in $J \cdot mol^{-1}$ for O_2 and CO_2, respectively. M_i symbolises mass of the produce i in kg. For simplicity, we assume that each cell in a produce has the same mass. $rO2$ and $rCO2f$ corresponds to the preexponential factor for produce respiration and fermentation in $mL \cdot kg^{-1} \cdot hr^{-1}$. $ErO2$ and $ErCO2f$ represent the respiration and fermentation activation energy for the produce expressed in $J \cdot mol^{-1}$.

Stage 1 (diffusion between package and external environment):

$\forall \alpha = 1, \ldots, d$

diffusion rule D_α	conditions	action
$[\sigma] \to []\sigma$	$(\sigma \in S) \wedge (\{(\sigma, f_\alpha)\} \subseteq L_t)$	$L_t := L_t \ominus \{(\sigma, f_\alpha)\}$
$[]\sigma \to [\sigma]$	$(\sigma \in S)$	$L_t := L_t \uplus \{(\sigma, f_\alpha)\}$

with $f_\alpha(L_t) = \left\lfloor k_\alpha(G) \cdot \Delta\tau \cdot \hat{\mathrm{f}}(|L_t \cap \{(\sigma, \infty)\}|) \right\rfloor$

Stage 2 (diffusion between plant cells and package):

$\forall i = 1, \ldots, m$
$\quad \forall \alpha = 1, \ldots, d_i$

diffusion rule $D_{i,\alpha}$	conditions	action
$[\sigma]_{cell_{i,j}} \to []_{cell_{i,j}}\sigma$	$(\sigma \in S) \wedge (cell_{i,j} \in N_i) \wedge$ $(\{(\sigma, f_{i,\alpha})\} \subseteq L_{i,j,t})$	$L_{i,j,t} := L_{i,j,t} \ominus \{(\sigma, f_{i,\alpha})\}$ $L_t := L_t \uplus \{(\sigma, f_{i,\alpha})\}$
$[]_{cell_{i,j}}\sigma \to [\sigma]_{cell_{i,j}}$	$(\sigma \in S) \wedge (cell_{i,j} \in N_i) \wedge$ $(\{(\sigma, f_{i,\alpha})\} \subseteq L_t)$	$L_t := L_t \ominus \{(\sigma, f_{i,\alpha})\}$ $L_{i,j,t} := L_{i,j,t} \uplus \{(\sigma, f_{i,\alpha})\}$
$[\sigma]_{cell_{i,j}} \to [\sigma]_{cell_{i,k}}$	$(\sigma \in S) \wedge (k \neq j) \wedge (cell_{i,j} \in N_i) \wedge$ $(cell_{i,k} \in N_i) \wedge ((cell_{i,j}, cell_{i,k}) \in E_i)$ $\wedge (\{(\sigma, f_{i,\alpha})\} \subseteq L_{i,j,t})$	$L_{i,j,t} := L_{i,j,t} \ominus \{(\sigma, f_{i,\alpha})\}$ $L_{i,k,t} := L_{i,k,t} \uplus \{(\sigma, f_{i,\alpha})\}$

with $f_{i,\alpha}(L_t) = \left\lfloor k_{i,\alpha}(G, G_i) \cdot \Delta\tau \cdot \hat{\mathrm{f}}(|L_t \cap \{(\sigma, \infty)\}|) \right\rfloor$

Stage 3 (reactions occurring within each cell):

$\forall i = 1, \ldots, m$
$\quad \forall j = 1, \ldots, n_i$
$\quad\quad \forall \alpha = 1, \ldots, r_{i,j}$

reaction rule $R_{i,j,\alpha}$	conditions	action
$(A_{i,j,\alpha}, B_{i,j,\alpha})$	$f_{i,j,\alpha} \cdot A_{i,j,\alpha} \subseteq L_{i,j,t}$	$L_{i,j,t} := L_{i,j,t} \ominus f_{i,j,\alpha} \cdot A_{i,j,\alpha}$ $\uplus f_{i,j,\alpha} \cdot B_{i,j,\alpha}$

with $f_{i,j,\alpha}(L_{i,j,t}) = \left\lfloor k_{i,j,\alpha}(G, G_i) \cdot \Delta\tau \prod_{\substack{\forall c \in \mathrm{supp}(A_{i,j,\alpha}) : \\ (R_{i,j,\alpha} = (A_{i,j,\alpha}, B_{i,j,\alpha}))}} \hat{\mathrm{f}}(|L_{i,j,t} \cap \{(c, \infty)\}|)^{|A_{i,j,\alpha} \cap \{(c,\infty)\}|} \right\rfloor$

Increment time t:

$L_{t+1} := L_t$
$\forall i = 1, \ldots, m$
$\quad \forall j = 1, \ldots, n_i$
$\quad\quad L_{i,j,t+1} := L_{i,j,t}$

Fig. 2. Iteration scheme for the temporal evolution of Π_{MAP} system

Most of the values for these symbols were taken from the literature [4]. Symbols $O2, CO2, H2O$, $Ethanol$ and $Glucose$ represent amounts of species O_2, CO_2, H_2O, Ethanol and Glucose. Initial values for these symbols in each compartment and the rest of the parameters were assigned empirically.

$$
\begin{aligned}
S &= \{CO2, Ethanol, Glucose, H2O, O2\} \\
G &= \{M, T, R, A, E, CO2ex, H2Oex, O2ex, EaCO2, EaO2, pCO2, pO2, pH2O\} \\
N_1 &= \{cell_{1,1}, cell_{1,2}, cell_{1,3}\} \\
N_2 &= \{cell_{2,1}\} \\
G_i &: \{ErO2, rO2, ErCO2f, rCO2f\} \ \forall i \in \{1,2\} \\
D_1 &: []_{package} O2 \rightleftharpoons [O2]_{package} \\
\mathrm{f}_1(L_t) &= \left\lfloor \frac{A}{E} \cdot (\mathrm{O2ex} - \mathrm{L_t(O2)}) \cdot pO2 \cdot e^{\frac{-EaO2}{R \cdot T}} \right\rfloor \\
D_2 &: [CO2]_{package} \rightleftharpoons []_{package} CO2 \\
\mathrm{f}_2(L_t) &= \left\lfloor \frac{A}{E} \cdot (\mathrm{L_t(CO2)} - \mathrm{CO2ex}) \cdot pCO2 \cdot e^{\frac{-EaCO2}{R \cdot T}} \right\rfloor \\
D_3 &: [H2O]_{package} \rightleftharpoons []_{package} H2O \\
\mathrm{f}_3(L_t) &= \left\lfloor \frac{A}{E} \cdot (\mathrm{L_t(H2O)} - \mathrm{H2Oex}) \cdot pH2O \right\rfloor \\
D_{1,1} &: []_{cell_{1,1}} O2 \rightleftharpoons [O2]_{cell_{1,1}} \qquad \mathrm{f}_{1,1}(L_t) = k_{1,1} \cdot L_t(\mathrm{O2}) \\
D_{1,2} &: [CO2]_{cell_{1,1}} \rightleftharpoons []_{cell_{1,1}} CO2 \qquad \mathrm{f}_{1,2}(L_t) = k_{1,2} \cdot L_t(\mathrm{CO2}) \\
D_{1,3} &: [H2O]_{cell_{1,1}} \rightleftharpoons []_{cell_{1,1}} H2O \qquad \mathrm{f}_{1,3}(L_t) = k_{1,3} \cdot L_t(\mathrm{H2O}) \\
D_{1,4} &: [O2]_{cell_{1,1}} \rightleftharpoons [O2]_{cell_{1,2}} \qquad \mathrm{f}_{1,4}(L_t) = k_{1,4} \cdot L_t(\mathrm{O2}) \\
D_{1,5} &: [CO2]_{cell_{1,2}} \rightleftharpoons [CO2]_{cell_{1,1}} \qquad \mathrm{f}_{1,5}(L_t) = k_{1,5} \cdot L_t(\mathrm{CO2}) \\
D_{1,6} &: [H2O]_{cell_{1,2}} \rightleftharpoons [H2O]_{cell_{1,1}} \qquad \mathrm{f}_{1,6}(L_t) = k_{1,6} \cdot L_t(\mathrm{H2O}) \\
D_{1,7} &: [O2]_{cell_{1,2}} \rightleftharpoons [O2]_{cell_{1,3}} \qquad \mathrm{f}_{1,7}(L_t) = k_{1,7} \cdot L_t(\mathrm{O2}) \\
D_{1,8} &: [CO2]_{cell_{1,3}} \rightleftharpoons [CO2]_{cell_{1,2}} \qquad \mathrm{f}_{1,8}(L_t) = k_{1,8} \cdot L_t(\mathrm{CO2}) \\
D_{1,9} &: [H2O]_{cell_{1,3}} \rightleftharpoons [H2O]_{cell_{1,2}} \qquad \mathrm{f}_{1,9}(L_t) = k_{1,9} \cdot L_t(\mathrm{H2O}) \\
D_{2,1} &: []_{cell_{2,1}} O2 \rightleftharpoons [O2]_{cell_{2,1}} \qquad \mathrm{f}_{2,1}(L_t) = k_{2,1} \cdot L_t(\mathrm{O2}) \\
D_{2,2} &: [CO2]_{cell_{2,1}} \rightleftharpoons []_{cell_{2,1}} CO2 \qquad \mathrm{f}_{2,2}(L_t) = k_{2,2} \cdot L_t(\mathrm{CO2}) \\
D_{2,3} &: [H2O]_{cell_{2,1}} \rightleftharpoons []_{cell_{2,1}} H2O \qquad \mathrm{f}_{2,3}(L_t) = k_{2,3} \cdot L_t(\mathrm{H2O}) \\
R_{i,j,1} &: Glucose + 6\ O2 \rightarrow 6\ CO2 + 6\ H2O\ \ \forall i \in \{1,2\} \wedge j \in \{1,2,3\} \\
\mathrm{f}_{i,j,1}(L_{i,j,t}) &= \left\lfloor \frac{L_{i,j,t}(Glucose)}{\Theta_{i,j,1,1} + L_{i,j,t}(Glucose)} \cdot \frac{L_{i,j,t}(\mathrm{O2})^6}{\Theta_{i,j,1,2} + L_{i,j,t}(\mathrm{O2})^6} \cdot \frac{M_i}{3} \cdot rO2 \cdot e^{\frac{-ErO2}{R \cdot T}} \right\rfloor \\
R_{i,j,2} &: Glucose \rightarrow 2\ Ethanol + 2\ CO2\ \ \forall i \in \{1,2\} \wedge j \in \{1,2,3\} \\
\mathrm{f}_{i,j,2}(L_{i,j,t}) &= \left\lfloor \frac{L_{i,j,t}(\mathrm{Glucose})}{\Theta_{i,j,2,1} + L_{i,j,t}(\mathrm{Glucose})} \cdot M_i \cdot rCO2f \cdot e^{\frac{-ErCO2f}{R \cdot T}} \right\rfloor
\end{aligned}
$$

Figure 3 shows the corresponding courses of $plant_1$ internal gas composition, resulting from following parameter setting for the discrete iteration scheme: $A = 100$, $E = 1$, $M_i = 0.1$, $pO2_i = 1620000$, $EaO2_i = 43100$, $pCO2_i = 238000$, $EaCO2_i = 34300$, $rO2_i = rCO2f_i = 3 \times 10^{14}$, $ErO2_i = ErCO2f = 70700$, $pH2O_i = 1$, $\Theta_{i,j,1,k} = 1$, for $i \in \{1,2\}$ and $j \in \{1,2,3\}$ and $k \in \{1,2\}$; $k_{1,j} = 0.2$ for $j \in \{1,\ldots,9\}$, $k_{2,j} = 0.2$ for $j \in \{1,\ldots,3\}$. A fixed value $T = 277.15$ was considered for a constant temperature scenario, and transient values for $273.15 \leq T \leq 293.15$ were obtained through a sigmoid function to represent changes in temperature over time in another scenario. Simulations have been performed using Copasi [12]. Differences in internal gas composition of $plant_1$ have been observed

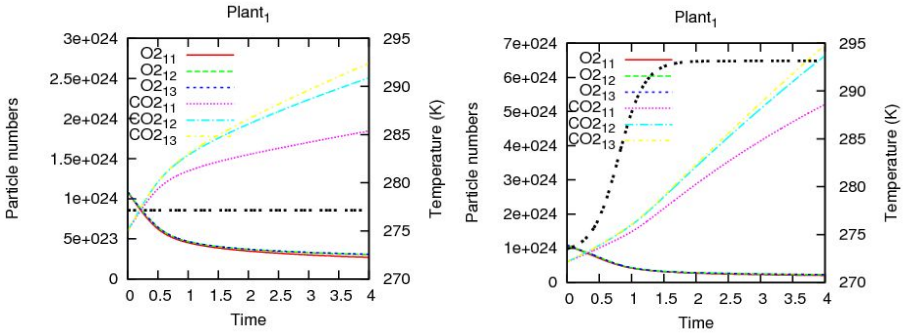

Fig. 3. Dynamical behaviour for gas composition for $plant_1$ in constant and varying temperature scenarios

during time due to the interplay between cellular respiration and fermentation processes and intercellular diffusion. Those differences could determine the form of maturation of the produce, in this case, from the center to the skin. An equilibrium is reached in the package gas composition, while respiration rates of the produces diminished.

5 Conclusions

Using a membrane based model for MAP, we presented a framework that is able to abstract packaging for different fruit and vegetable types, varieties or developmental stages. Respiration of the produce is considered as the basic process when modelling MAP, and predictions about the dynamical behaviour of such systems can be improved taking into account environmental, biological and technical factors. Our approach allows extensions including other low level processes, such as ethylene signaling pathway, cell/tissue rupture due to produce cutting and transport of other molecules, that can been advantageously modeled using P systems.

Finally, the quality of the packaged produce (taste, odour, texture, colour and appearance) is based on some subjective consumer evaluation. These traits are based on specific product properties, such as sugar content, volatile production and cell wall structure [19], and therefore can be introduced into the model through reactions, as a mechanism to obtain more knowledge about the impact of packaging conditions over product quality.

Considering texture (softening) of the fruit or vegetable, a next extension of this model will include cell wall structure contents and reactions. To do so, we plan to add a new membrane surrounding the structure on the cell level in order to represent this compartment, and a new stage in the evolution algorithm. Also, dissolution rules can be defined in this framework to capture cell wall dissolution. Additionally, to perform further simulations, we plan to implement the model in P-Lingua [6], basically because ODE-based simulators for membrane systems are unable to deal with structural changes.

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