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A decision support system to optimize fresh food packaging

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Abstract. *Preserving fresh fruits and vegetables after harvest and during further storage is an important issue in the food industry. Beyond respect of the chill chain, modified atmosphere is an efficient way to delay senescence and spoilage without using controversial preservatives compounds or technologies. Modified atmosphere packaging (MAP) relies on modification of the atmosphere inside the package in order to extend food shelf life by reducing physiological degradation rate. MAP is achieved by the interplay of two processes: (1) the transfer of gases through the packaging and (2) the respiration of the product. MAP can be achieved by matching the film permeation rate (namely O₂ and CO₂ permeabilities) with the respiration rate of the product. A mathematical model (www.tailorpack.com) has been developed to design MAP for fresh fruits and vegetables. Such numerical tool simplify the package design steps by allowing to predict in advance the required window of packaging permeability for maintaining the quality and safety of the packed food. However, such a mathematical model required several input parameters such as maximal respiration rates that are obtained from experimental data and are characterized by high uncertainties due to the biological variation. Although uncertainty propagation during MAP modeling presents significant concerns, this subject has been seldom considered. It would be nevertheless indispensable to consider it in the development of a complete decision support system for the design of fresh products packaging.*

In this work, we present a complete decision support system (DSS) that aims at helping decision makers to find the best packaging material for a given fruit or vegetable. This DSS is composed of two distinct parts. The first part consists in an optimization system that uses the MAP mathematical model and food parameters to determine optimal permeabilities of packaging. In order to integrate existing uncertainties in the study and still keep a reasonable time to perform the optimization task, we propose to use an approach based on interval analysis rather than the more classical probabilistic approach. The approach has the advantage to make a minimal amount of assumption and to require only a few evaluations of the model. The results of this uncertainty studies are optimal values of permeabilities described by fuzzy sets. The second part of the DSS consists in a database where is stored information concerning various packaging material. The system considers, among other criteria, fuzzy sets obtaining in the first part to interrogate the database, and can consider other user preferences expressed by fuzzy sets (i.e., gradual preferences). It allows to differentiate between compulsory requirements (i.e. that the users absolutely wants to be satisfied) and desirable requirements (i.e. that users would like to satisfy, if possible).

Keywords. Fresh food packaging, reverse engineering, optimization under uncertainty, flexible database querying, multi criteria decision, fuzzy sets

Introduction

Modified atmosphere packaging (MAP) of fresh fruits and vegetable relies on the modification of the atmosphere inside the package in order to extend the food shelf life by reducing the respiration of the product and consequently its degradation rate. Atmosphere composition within the package is the result of both respiration of the commodity and diffusion/permeation of gases through the film until a steady modified atmosphere is reached (Floros and Matsos 2005). This steady atmosphere should be close to an optimal gas concentration specific to each product. Hence, gas transfer properties of the packaging must correctly match physiological requirements of the product (SEQ).

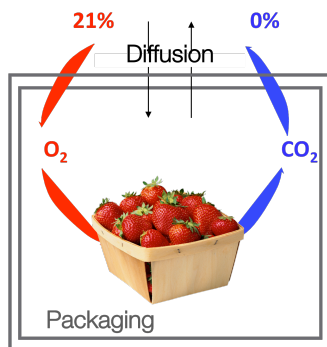


Figure 1: Schema of the food/packaging system illustrating O_2 and CO_2 gas exchange

In order to design MAP for fresh fruits and vegetables, mathematical models have been developed to simulate the evolution of internal gas composition in the packaging as a result of food respiration and mass transfer through the packaging material (Charles, Sanchez et al. 2003; Mahajan, Oliveira et al. 2007). When optimal gas composition for a fruit or vegetable is known, these models can be used to find optimal gas permeabilities. These models include several input parameters such as film thickness, area, mass of packed vegetables and, of course, the respiration characteristics of the product, i.e. parameters of the Mickaëlis-Menten equation.

These parameters, and especially respiration parameters, are obtained from experimental data and are characterized by high uncertainties due to the biological variation (Hertog, Scheerlinck et al. 2007). Although these uncertainties can considerably impact optimization steps and model prediction reliability, their handling has been seldom addressed in MAP design and more generally in food engineering. We can nevertheless mention the works of (Baudrit, Helias et al. 2009) who studied the impact of variability and uncertainty propagation in the modeling of cheese mass during ripening and the works of (Hertog et al. 2007) who evaluated the impact of biological variation on vegetables postharvest behavior. Both teams used classical probabilistic methods (Bedford and Cooke 2001) in their uncertainty handling (either as a unique framework or as part of a hybrid framework). Note that such methods require to (i) know and specify the distribution of each input variable (e.g. normality), (ii) specify the dependency structures between input variables and (iii) perform (costly) numerical analysis to evaluate the output uncertainty (Monte Carlo simulation technique). Note that the third point is particularly critical for on-line decision support systems.

An alternative to costly Monte Carlo simulations is to use interval analysis (Jaulin, Kieffer et al. 2001) to perform the uncertainty analysis. Interval analysis only requires to specify the bounds in which each input variables and parameters may vary, and makes no assumption about variable dependencies. Compared to probabilistic analysis, interval analysis can therefore be seen as a conservative analysis, in the sense that it needs a minimal amount of information about variables, and possibly ignore some of it when available. In our context, the use of interval analysis allows us (i) to make safe in recommendation about optimal permeabilities and (ii) to use efficient computational methods, therefore allowing for fast on-line computations.

The MAP model handling uncertainty is included in a Decision Support System (DSS) whose objective is to select the packaging material that best suits a user needs. The DSS is a database of packaging material, interrogated by the means of flexible bipolar querying techniques. Flexible means that preferences can be gradual, i.e., different satisfaction levels between totally satisfied and unsatisfied are allowed. This is modeled by the means of fuzzy sets. Bipolar means that queries can be composed of both negative and positive preferences. Negative preferences are constraints (e.g. gas transfer properties of the packaging must match the physiological requirements of the product), while

positive preferences are wishes (e.g. packaging material with minimal cost, etc). While objects not satisfying negative preferences are definitely rejected, objects not satisfying positive preferences are just deemed as less desirable than others.

This paper presents (1) the MAP mathematical model used to predict optimal permeabilities, (2) the interest of interval analysis to achieve uncertainty analysis on the MAP model (and on models in general) and (3) a description of the Decision Support System.

MAP modeling

In modified atmosphere packaging, oxygen and carbon dioxide partial pressures in packaging headspace are modified and settle to steady values after a transient phase. This modification in the internal gases partial pressures is achieved due to the mass balance between oxygen and carbon dioxide flux through the packaging material and O₂ and CO₂ consumption/ production due to the product respiration.

$$p_{O_2}^{pkg} = \frac{Pe_{O_2} \cdot S}{e} (p_{O_2}^{ext} - p_{O_2}^{pkg}) - RR_{O_2} \cdot m = f_1 \quad \text{Equation 1}$$

$$p_{CO_2}^{pkg} = \frac{Pe_{CO_2} \cdot S}{e} (p_{CO_2}^{ext} - p_{CO_2}^{pkg}) + RR_{O_2} \cdot m \cdot RQ = f_2 \quad \text{Equation 2}$$

with

$$RR_{O_2} = \frac{RR_{O_2 \max} \cdot p_{O_2}^{pkg}}{(K_{m_{appO_2}} + p_{O_2}^{pkg}) \cdot (1 + p_{CO_2}^{pkg} / K_{iCO_2})} \quad \text{Equation 3}$$

where the first part of the right-hand side of f_1 and f_2 describes gas flux per time unit through the packaging material, while the second part describes gas consumption (and emission) by the vegetable or fruit (modelled using a Michaëlis-Menten-type equation).

SEQ summarises the parameters and sign of f_1 and f_2 partial derivatives w.r.t. each of its parameters.

For a given fruit or vegetable, it is possible to experimentally determine (up to some uncertainties) oxygen and carbon dioxide partial pressures that will result in an optimal preservation. From these values, it is then possible to identify optimal packaging permeabilities, by using identification algorithm on the mathematical model given by Eq. (1)-(3). SEQ shows a simulation realized using the web-application (www.tailorpack.com) without including uncertainties.

Determining exactly the values of the various parameters (S , e , $RR_{O_2 \max}$, etc) involved in Eq. (1) to (3) is a difficult task.

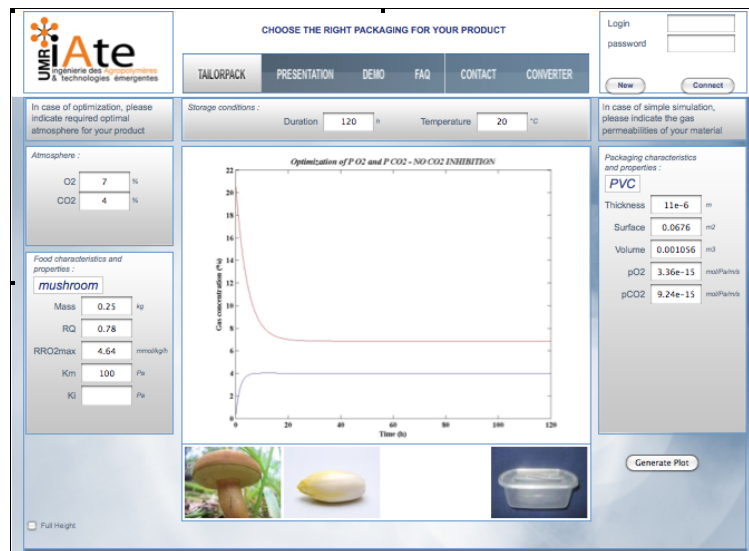


Figure 2: Example of simulation carried on the web-application www.tailorpack.com to identify the optimal gas permeabilities for a targeted fresh product

Table 1: Input parameters required for the MAP mathematical model

Parameter	Name	Units	f_1	f_2
Pe_{O_2}	O ₂ permeability	mol.m ⁻¹ .s ⁻¹ .Pa ⁻¹	↗	×
Pe_{CO_2}	CO ₂ permeability	mol.m ⁻¹ .s ⁻¹ .Pa ⁻¹	×	↘
S	Packaging surface	m ²	↗	↘
e	Packaging thickness	m	↘	↗
p_j^i	Partial pressure of j in i	kPa	↘	↘
RR_{O_2}	O ₂ respiration rate	mmol.kg ⁻¹ .h ⁻¹	↘	↗
$RR_{O_2 \max}$	Max. O ₂ respiration rate	mmol.kg ⁻¹ .h ⁻¹	↘	↗
$K_{m_{app}O_2}$	Mickaëlis-Menten constant	kPa	↗	↘
K_{iCO_2}	CO ₂ inhibition constant	kPa	↘	↗
m	mass of food	kg	↘	↗
RQ	Respiration quotient	(-)	×	↗

In practice, only handful measurements are performed and parameters values are imprecisely known. Including these uncertainties in the optimization step would provide more reliable and robust estimation.

Interval analysis and error propagation during MAP modeling

Basics of interval analysis. In interval analysis, uncertainty around a parameter x is modelled by an interval $[x] = [x-, x+]$, with $x-$ and $x+$ the lowest and highest values of variable x . Performing interval analysis on a function $f: \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ then amounts to compute the bounds $f([x]) = \{f(x) | x \in [x]\}$.

Computing exactly such bounds may be difficult, but when $f: \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ satisfy some monotonicity properties, computation can be simplified by focusing on specific points. For example, if $f(x, y) = x + y$ and $x \in [2, 5]$, $y \in [3, 7]$, then $f([x], [y]) \in [5, 12]$, the two bounds 5 and 12 being obtained for $x = 2, y = 3$ and $x = 5, y = 7$, and all other possible values give an answer between 5 and 12. In this case, only two precise computations are needed to retrieve the bounds. A similar property applies to dynamical models made of ordinary differential equations whose partial derivatives w.r.t. one parameter always have the same sign. As this is the case of Eq. (1) to (3) (see Table 1), we can easily replace precisely valued parameters by intervals and evaluate the interval-valued solution of the dynamical system. This is done by concentrating on specific extreme combinations of the interval-valued parameters and variables (initial conditions) to compute lower and upper envelopes. See (Destercke and Guillard 2011b) for details.

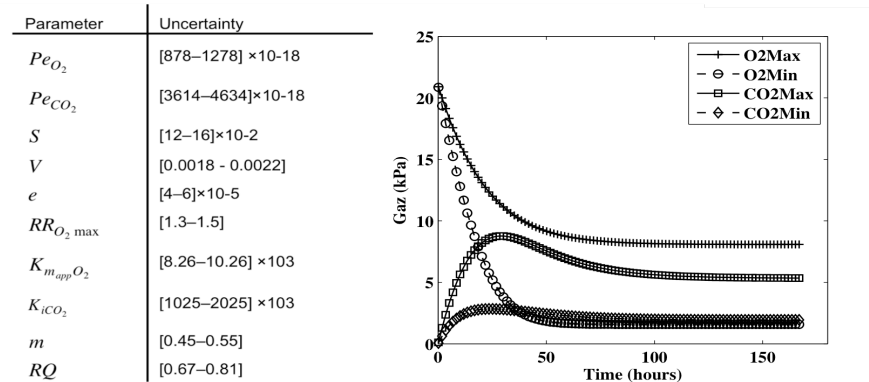


Figure 3: Uncertainty propagation during the modelling of modified atmosphere packaging of chicory packed in LDPE pouches. Input parameters are summarized on the right

Application to the case of chicory. Knowing the permeability of the packaging material classically used to pack chicory, the mathematical model described by Eq (1)-(3) can be used to simulate the evolution with time of the internal O₂ and CO₂ partial pressures. Parameters with their interval

uncertainty are summarised in SEQ. Maximal shelf life is estimated to be 7 days (i.e. simulation time about 200 hours). Figure 3 displays the result of interval analysis considering the uncertainty on all input model parameters (except the volume of headspace, shelf life and temperature). We can see that at steady state the O_2 level in the packaging varies between 1.6 and 8.1. This means that MAP experiments with similar conditions should result in experimental O_2 and CO_2 measurements included in these bounds. Recall that they are conservative bounds, and that better ones could be obtained using additional information. However, with this methodology, only four simulations were needed (two for each gas) to estimate the bounds.

As in the precise case, the results of interval propagation can be used to identify optimal O_2 and CO_2 permeabilities for a given fruit or vegetable. To do so, optimal and possibly interval-valued oxygen and carbon dioxide concentrations have to be specified. Optimisation then requires to differentiate two type of optimal solutions (a solution is a pair of O_2 and CO_2 permeability values): guaranteed solutions, for which we are certain that the true answer lies within the optimal O_2 and CO_2 concentrations; and possible solutions, for which the true answer may or may not lies within the optimal O_2 and CO_2 concentrations. Possible solutions have gradual satisfaction degrees for the designer. In the case of chicory, we consider that required O_2 and CO_2 partial pressures at equilibrium should be between 4 and 10 % for O_2 and 2 and 5 % for CO_2 , the guaranteed solutions (those have maximal value 1 in Figure 4) ranged from 1.59 to $1.92 \times 10^{-15} \text{ mol.m}^{-1}.\text{s}^{-1}.\text{Pa}^{-1}$ and 4.94 to $7.50 \times 10^{-15} \text{ mol.m}^{-1}.\text{s}^{-1}.\text{Pa}^{-1}$ for respectively O_2 and CO_2 permeability. Possible and non-guaranteed solutions (between 0 and 1 on Figure 4), ranged from 0.34 and $4.34 \times 10^{-15} \text{ mol.m}^{-1}.\text{s}^{-1}.\text{Pa}^{-1}$ and 1.78 to $19.96 \times 10^{-15} \text{ mol.m}^{-1}.\text{s}^{-1}.\text{Pa}^{-1}$.

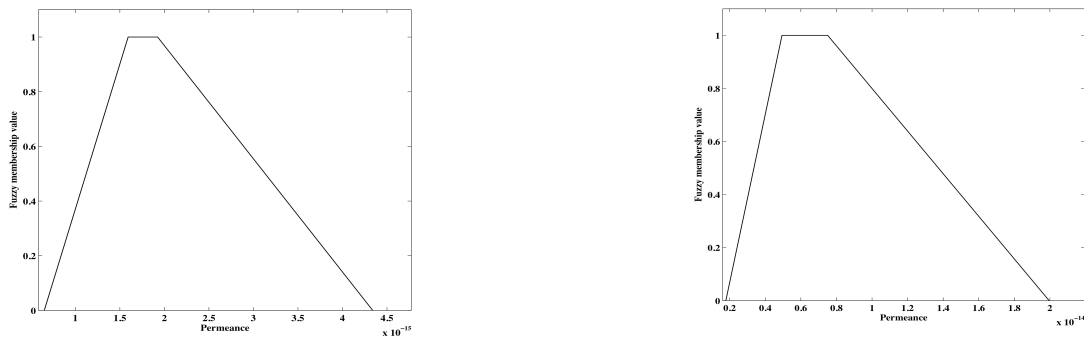


Figure 4: Optimal O_2 (left) and CO_2 (right) permeability range obtained by optimisation of the MAP model under interval uncertainty. Guaranteed solutions correspond to values with a maximal note of 1 and possible but not guaranteed solutions correspond to values with a note in $[0, 1]$

A new decision support system for food packaging design

In this section, we present a new decision support system (DSS) for fresh fruits and vegetables packaging design in which the flexible bipolar querying approach developed by the authors (Destercke et al 2011a) plays a central role. Optimisation using the MAP mathematical model only allows to give best preferred values for two (important) criteria: O_2 and CO_2 permeabilities that will best preserve food. However, for a sustainable design, several others criteria (economical, environmental, societal) must be satisfied depending on the acceptances, preferences and needs of all the involved stakeholders of the field, e.g., consumers, industry, environmental organizations ... Examples include the cost of the packaging material

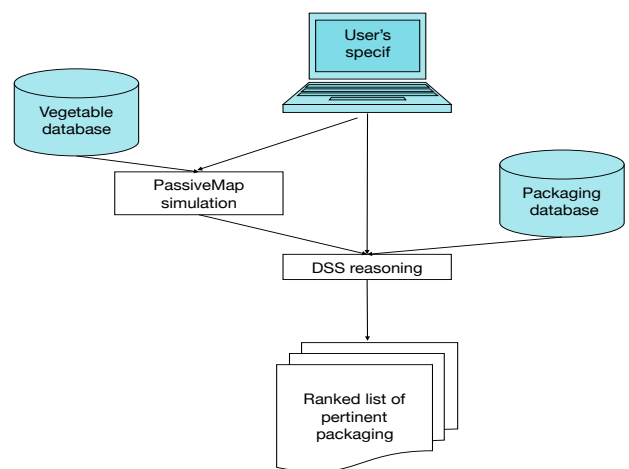


Figure 5: Global architecture of the DSS

(economical), the biodegradability of the packaging material (environmental), the reject of the use of some additives or nano-technology or simply the preference for transparent films (societal).

In our DSS (Figure 5), starting from a given fruit or vegetable, the user specifies its needs and preferences in terms of several criteria (e.g., conservation temperature, transparency, material cost). The system then queries the database and gives to the user an ordered list of materials that best suits his/her needs and preferences. Fuzzy modeling allow for some graduality in the specified preferences, while bipolar modeling gives the user the possibility to specify what criteria must be considered as constraints and what other criteria will be used to refine the ranking of the packaging materials that satisfy the constraints.

Starting from a vegetable/fruit specified by the user, the system scans a vegetable/fruit database to retrieve the parameter used to find optimal O₂ and CO₂ permeabilities. Using the targeted optimal O₂ permeability and the other user's requirements about criteria of various types, a query is then executed against the packaging database using the flexible bipolar querying engine. A list of ordered packaging materials is finally presented to the user.

Conclusions

The impact of uncertainty on input parameters was shown to be of high importance in the design of MAP. A simple method based on interval analysis was used instead of time consuming Monte Carlo simulations to determine the envelopes (i.e. extreme bounds) of the prediction. A first prototype of a Decision Support System (DSS) was presented able to provide multi-criteria decision in the domain of fresh food packaging on a base of constraints and wishes specified by the user.

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