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ABSTRACT

In this paper, we present the implementation of a dedicated software, MAP-OPT, for optimising the design of Modified Atmosphere Packaging of refrigerated fresh, non-respiring food products. The core principle of this software is to simulate the impact of the dynamic of gas (O$_2$/CO$_2$) exchanges on the growth of gas-sensitive microorganisms in the packed food system. In its simplest way, this tool, associated with a data warehouse storing food, bacteria and packaging properties, allows the user to explore his/her system in a user-friendly manner by adjusting/changing the pack geometry, the packaging material and the gas composition (mixture of O$_2$/CO$_2$/N$_2$). Via the @Web application, the data warehouse associated with MAP-OPT is structured by an ontology, which allows data to be collected and stored in a standardized format and vocabulary in order to be easily retrieved using a standard querying methodology. In an optimisation approach, the MAP-OPT software enables to determine the packaging characteristics (e.g. gas permeability) suitable for a target application (e.g. maximal bacterial population at the best-before-date). These targeted permeabilities are then used to query the packaging data warehouse using the @Web application which proposes a ranking of the most satisfying materials for the target application, i.e. packaging materials whose characteristics are the closest to the target ones identified by the MAP-OPT software. This approach allows a more rational dimensioning of MAP of non-respiring food products by selecting the packaging material fitted to “just necessary” (and not by default, that with the greatest barrier properties). A working example of MAP dimensioning for a strictly anaerobic, CO$_2$-sensitive microorganism, *Pseudomonas fluorescens*, is proposed to highlight the interest of the software.

Keywords:

Software; Predictive microbiology; Modified Atmosphere Packaging; Ontology; Data warehouse; Mass transfer; Decision making strategy
1- Introduction

To design Modified Atmosphere Packaging (MAP) of non-respiring food products in order to ensure microbial safety and quality, numerous phenomena must be considered, the most important ones being the impact of O$_2$ and CO$_2$ and their exchange between the food and the packaging on microbial growth (Chaix, Broyart, et al., 2015; Chaix, Couvert, Guillaume, Gontard, & Guillard, 2015; Devlieghere et al., 2001; Simpson, Acevedo, & Almonacid, 2009; Simpson & Carevic, 2004). The gas mixture required for limiting microbial growth and the packaging material necessary to maintain an effective gas concentration are strongly dependent on the geometry of the system (e.g. volume of package, mass of food, etc.), the microbial flora, the gas permeation through the packaging material, the rate of gas dissolution and diffusion into the food product and of course the storage temperature. The complexity of the mechanisms implies that food manufacturers have to arbitrarily test several gas and packaging conditions until they find the most suitable combination for their target product and its expected shelf life. To do that, the food manufacturer first arbitrarily chooses his packaging material (mainly selected according to its cost and sealing ability) and then he packs his produce hoping that the right combination of packaging material, atmosphere and produce is in the set of his trials. If not, he starts a new set of experiments again. This empirical approach called “pack and pray” approach is very time and cost consuming, and with a high risk of failure (Floros and Matsos, 2005; Angellier-coussy et al., 2013). That's why it would be preferable to use a requirement driven approach in which the needs and requirements of the food would be the starting point (e.g. maximal bacterial load at the best-before-date) and then translated into packaging mass transfer properties. Once these properties are known, they are considered as constraints in the choice of the packaging material. This optimised approach relies on the use of mathematical modelling tools for which interest has already been demonstrated for respiring products such as fresh fruits and vegetables (Cagnon, Méry, Chalier, Guillaume, & Gontard, 2013; Guillard et al., 2015) but which have not yet been applied when microbial growth limitation prevails.
Predicting microbial safety in MAP requires taking into account among other parameters, such as temperature, food pH, Aw, salt content, etc., the dynamic of gas exchanges. However, this aspect, up to recent works (Chaix, Broyart, et al., 2015; Simpson, Almonacid, Acevedo, & Cortes, 2003) was never seriously considered. Even if existing tools of predictive microbiology – see for example the Sym’Previus software (Leporq, Membré, Dervin, Buche, & Guyonnet, 2005) or Combase tool (Baranyi & Tamplin, 2004) - consider in some cases CO₂ effect on microbial growth, it is always a value kept constant (e.g. the initial concentration flushed in the pack) and these tools never consider the O₂ effect on aerobe growth nor bacterial O₂ consumption and CO₂ production rate.

Different classes of microorganisms regarding their susceptibility/tolerance to oxygen and carbon dioxide can be distinguished. Oxygen can either be indispensable, facultative, or toxic for microbial growth. Except for anaerobes, reduction of the oxygen level usually causes metabolic modification and reduction of the growth rate. Contrary to oxygen, carbon dioxide is often considered as an inhibitor of microbial growth. But some microorganisms are relatively tolerant to moderate to high levels of CO₂ (Chaix et al. 2015b). Depending on these classes of microorganisms, MAP could be efficient or not.

In order to propose a software aiming at helping the food manufacturer to properly design his/her MAP system in the case of MAP-sensitive microorganisms, we have developed a semi-mechanistic model coupling O₂/CO₂ transfer equations and predictive microbiology models (Chaix, Broyart, et al., 2015). This model takes into account O₂/CO₂ permeation through the packaging material, the O₂/CO₂ dissolution/diffusion into the food product and the impact of O₂/CO₂ headspace partial pressure and gradient into food on the growth of O₂/CO₂ sensitive microorganisms. The effect of temperature on all phenomena, through Arrhenius law for mass transfer and cardinal model for microbial growth, is also included. This model was successfully validated on a simplified system, a model cheese, inoculated with *Listeria monocytogenes* (Chaix, Broyart, et al., 2015) and on real products, poultry meat and salmon, inoculated with *Listeria monocytogenes* – moderately sensitive to CO₂ (Augustin, Zuliani, et al., 2005) and highly tolerant to O₂, (Lungu, Ricke, & Johnson, 2009) – and/or *Pseudomonas fluorescens* – sensitive to both CO₂ and lack of O₂ – through dedicated challenge-tests (Guillard et al., 2016). In the present work, to improve this mathematical model in such a way that it provides real
decision variables and not only technical variables (such as permeation rate of $O_2$ or growth curves) which are insufficient to address decision, it has been coupled with a data warehouse containing food, bacteria and packaging characteristics and implemented in a user-friendly web interface, constituting the MAP-OPT software. Data are structured and stored in the data warehouse according to a unique and specific ontology dedicated to the food, bacteria and packaging fields. Part of these data includes the input parameters of the computer programme implementing the semi-mechanistic model (for instance, $O_2/CO_2$ solubilities and diffusivities into the food). Thanks to the available structure of the data, it is easy to re-use them in various simulations in the MAP-OPT software. The high number of data (more than 350 distinct packaging data are currently stored in the data warehouse) allows numerous and fruitful simulations to be realized.

When the packaging material is not predefined, the objective is to identify it, taking into account gas evolution and shelf life constraints. In that objective, the MAP-OPT software helps the user to determine the optimal packaging permeabilities for a given case study. Using these target permeability values and the @Web querying modulus (Buche, Dibie, Ibanescu, & Soler, 2011) that allow to explore and query the data warehouse, a ranking of the most suitable types of packaging is thus proposed to help the user to make his decision. Such unprecedented, original strategy combining computer simulations and database querying allows an integrated and reasoned approach for choosing the “just necessary” packaging material and not by default the most barrier one or the cheapest one.

The objective of this paper is to present the functionalities of the proposed MAP-OPT software and its associated ontology-guided data warehouse. A presentation of the software and the data warehouse structure, development and implementation are first proposed. Then examples of the pipeline of data and models starting from the definition of the system, going through computer simulations, identification of the packaging material and finally experimental validation of the solution proposed by the software is presented using the experimental pool of data obtained in dedicated challenge tests detailed in a previous work (Guillard et al., 2016).
2. DEVELOPMENT OF THE MAP-OPT TOOL

2.1. Data management

Data needed in the semi-mechanistic model for performing numerical simulations and decision support issues (e.g. food product respiration rate, O₂/CO₂ solubility and diffusivity, packaging O₂/CO₂ permeability, etc.) are numerous and consequently require a careful and structured organization in a data warehouse. Moreover, those data are coming from heterogeneous data sources (e.g. scientific papers, commercial packaging technical sheets), which are available in various formats (e.g. pdf, html, excel files). They can be incomplete, of variable reliability and expressed in different units of measure.

For all those reasons, the data management has to be guided by an ontology. An ontology is a description (such as a formal specification of a programme) of the concepts and relationships that can exist for a community of agents, in order to enable knowledge sharing and reuse (Gruber, 1993).

Moreover, the ontology designed for our data warehouse (Buche et al., 2011) can be used as a reading grid in order to help annotators to identify and extract from the original heterogeneous data sources relevant data for numerical simulation and for decision support issues. For instance, in Fig. 1, the O₂Permeability Relation concept represents an O₂ permeability measure (i.e. an O₂Permeability quantity concept) for a given packaging (i.e. a Packaging concept) and the set of parameters required for data reusability (i.e. Thickness, Temperature, Diff_Partial_Pressure, Relative_Humidity quantity concepts) which the annotator should find in the document. The current version of the data warehouse containing more than 1538 experimental measures is structured thanks to an ontology dedicated to mass transfer domain including 38 Relation concepts defining types of measurement (e.g. permeabilities, diffusivities) described by 55 quantities associated with 159 units of measure including conversion factors and 917 symbolic concepts representing studied objects (e.g. food matrices, packaging). This ontology and associated annotated data are available on the @Web platform at http://www6.inra.fr/cati-icat-atweb/Ontologies/Transmat.

As annotated data come from heterogeneous data sources and will be reused for decision support issues, assessing their reliability is an important feature. To reach this goal, a reliability model
(Destercke, Buche, & Charnomordic, 2013) was designed and implemented in the data warehouse. Reliability indicators are computed thanks to metadata associated with the document and expert judgement quotations associated with metadata values. Various different types of meta-information, summarized can be considered:

- meta-information on the data source itself: for instance the source type (e.g., scientific publication, technical report,…), the source reputation, citation data;

- meta-information related to means used to collect data. Such information is typically included in a section called material and method in papers based on experiments in Life Science, which thoroughly describes the experimental protocol and material. Some methods may be known to be less accurate than others, but still be chosen for practical considerations;

- meta-information related to statistical procedures: presence of repetitions, uncertainty quantification (variance, confidence interval), elaboration of an experimental design.

Fig. 2A shows the experts quotations associated with the criterion Source type taken into account by the reliability model. Fig. 2B shows the reliability indicators associated with a given scientific document. Reliability indicator values range from 1 (i.e. low reliability) to 5 (i.e. high reliability). In the example, low and high expectations of the reliability indicators are far apart: it reveals contradiction in the metadata quotations. In this example, the criterion Source type has a high quotation regarding the reliability in order to take into account that the document benefited from an external peer-review. On the contrary, the Criterion Repetition has a low quotation, as no repetition value means that annotated experimental data don’t provide any information about their variability.

Criteria values quotations determined by expert judgements are available on the @Web platform; for example, the value no (resp. yes) associated with the Criterion Repetition has for quotation not at all reliable (resp. very reliable). The reliability model is flexible. Experts quotations associated with criteria may be modified if necessary. In this case, all indicators assessing document’s reliability are automatically updated. Moreover, the set of indicators can be extended if other dimensions of reliability must be taken into account (by example to take into account the accuracy of the method used to measure permeability). As shown in the use case of section 4 and in Fig. 8B, those indicators
enrich the packaging solution recommended by the decision support system providing a synthetic overview of the associated data reliability.

2.2. Computer programme describing food safety evolution

The mathematical model that simulates the evolution of gas and microbial growth in the MAP system has already been extensively detailed and validated in previous works (Chaix, Broyart, et al., 2015; V. Guillard et al., 2016). It models several physical and biological mechanisms occurring in the food/packaging system (e.g. food packed in a tray sealed by a lid film, Fig. 3). Mechanisms included in the semi-mechanistic model are (1) O₂/CO₂/N₂ permeation through the packaging material, (2) O₂/CO₂ solubilisation, (3) diffusion within the food, (4) microbial growth, (5) O₂/CO₂ consumption/production by the microbial flora (respiration), (6) variations in headspace volume and composition and (7) temperature effect on all the aforementioned phenomena.

(1) Fick’s first law was used to model permeation of gases through the packaging: mass transfer is considered mono-directional through the lid film and in a steady state regime. Mass transfer through the bottom of the tray was assumed to be negligible because of being in contact with the shop shelf. Mass transfer through the lateral faces of the tray in contact with headspace is included when necessary.

(2) & (3) Fick’s second law was used to represent transient diffusion of gases within the food. The flux was supposed to be mono-directional coming through the headspace toward the food surface. The correlation between gas partial pressure into headspace and concentration of dissolved gas at food interface was supposed to obey Henry’s law.

(4) Microbial growth was modelled using previously validated equations of predictive microbiology (Leporq, Membré, et al., 2005).

(5) The production/consumption of gases into headspace, principally due to the respiration of microorganisms was modelled using the semi-mechanistic Michaëlis-Menten equation (Fonseca, Oliveira & Brecht, 2002) based on a previous work carried out on Pseudomonas spp. by Thiele, Kamphoff, & Kunz (2006). The net consumption of O₂ depends on bacterial load, which of course,
varies as a function of time. Respiration law and microbial growth are thus strongly coupled. If respiration is negligible for a short storage time when the bacterial load is low, it could not be neglected anymore for long storage time when the bacterial load is high enough (> $10^3 - 10^4$ CFU/g) to significantly impact the gas composition in headspace (Guillard et al., 2016; Thiele et al., 2006).

(6) Variations in headspace volume and composition were assumed to obey the perfect gas law, total pressure remaining constant and equal the atmospheric pressure.

(7) Dependence on temperature according to Arrhenius equation was considered for permeation, diffusion, solubilisation and gas production/consumption. Dependence on temperature for microbial growth is considered through cardinal models (see § hereafter).

Details about the Partial Differential Equations used are given hereafter in the case of a negligible mass transfer through the tray sides corresponding to scheme provided in Fig. 3.

**a- Mass balance in packaging headspace**

One of the technical outputs of the mathematical simulation is the balance of gases (O$_2$, CO$_2$, N$_2$) in the headspace changing according to incoming, outgoing and production flux. This balance of gases is computed as follows:

$$V_{HS} \frac{dC_{j,HS}}{dt} + C_{j,HS} \frac{dV_{HS}}{dt} = \varphi_{j,L} + \varphi_{j,I} + S_{j,F}$$

where $C_{j,HS}$ stands for the concentration of gas species $j$ (O$_2$, CO$_2$ and N$_2$) in the headspace (kg m$^{-3}$), $V_{HS}$ is the volume of headspace (m$^3$), $\varphi_{j,L}$ is the mass flow (kg s$^{-1}$) of species $j$ occurring by permeation from the surrounding atmosphere to the headspace, $\varphi_{j,I}$ is the mass flow (kg s$^{-1}$) of species $j$ (O$_2$, CO$_2$) at the interface between the food sample and headspace due to solubilisation and diffusion and $S_{j,F}$ is the net production rate (kg s$^{-1}$) of species $j$ (O$_2$, CO$_2$) produced by biological reactions, if any, occurring within the food sample during conservation. We supposed that N$_2$ does not dissolve in the food product therefore only $\varphi_{j,I}$ for O$_2$ and CO$_2$ was considered.

The gas mixture in the headspace obeys the ideal gas law and the total pressure in the headspace $P_T$ remains constant during conservation and equal to atmospheric pressure:
\[ RT \sum_{j=[O_2, CO_2, N_2]} \frac{C_{j,HS}}{M_j} = P_T = 10^5 \text{ Pa} \] (2)

Therefore, headspace volume varies according to headspace composition and \( dV_{HS}/dt \) can be calculated as a pondered sum of the different aforementioned mass flow \( \varphi_{j,L}, \varphi_{j,I} \) and source terms \( S_{j,F} \) as follows:

\[
\frac{dV_{HS}}{dt} = RT \left( \frac{\varphi_{O_2,L} + \varphi_{O_2,I} + S_{O_2,F}}{M_{O_2}} + \frac{\varphi_{CO_2,L} + \varphi_{CO_2,I} + S_{CO_2,F}}{M_{CO_2}} + \frac{\varphi_{N_2,L}}{M_{N_2}} \right) \] (3)

where \( R \) is the ideal gas law constant \((=8.314 \text{ J mol}^{-1} \text{ K}^{-1})\), \( T \) the temperature (K) and \( M_{O_2}, M_{CO_2} \) and \( M_{N_2} \) the molar mass (kg mol\(^{-1}\)) respectively for O\(_2\), CO\(_2\) and N\(_2\).

**b- Mass flow of gaseous species through the lid film**

The mass flow \( \varphi_{j,L} \) (kg s\(^{-1}\)) of gas species \( j \) (O\(_2\), CO\(_2\) and N\(_2\)) through the lid film are calculated, using Fick’s first law and assuming a steady state regime for mass transfer through the film:

\[ \varphi_{j,L} = M_j Pe_j \left( \frac{A_L}{e_L} \right) \left( p_{j,\infty} - p_{j,HS} \right) \] (4)

where \( A_L \) (m\(^2\)) and \( e_L \) (m) are respectively the lid film surface and thickness, \( Pe_j \) (mol m\(^{-1}\) s\(^{-1}\) Pa\(^{-1}\)) is the permeability of gas species \( j \) through the film and \( p_{j,\infty} \) and \( p_{j,HS} \) (Pa) are respectively the partial pressure of species \( j \) in the surrounding atmosphere and in the headspace with, according to the ideal gas law assumption, \( p_{j,HS} = C_{j,HS}RT/M_j \). When mass transfer through the lateral faces of the tray is considered (which is systematically the case in the on-line tool), \( \varphi_{j,L} \) is calculated using \( Pe_j \), \( e \) and \( A \) as the result of the linear combination of values for the lid and the tray respectively, with respect to percentage of lid and lateral faces surface to the total packaging surface (for example, \( Pe_j = \text{ratio\_area\_lid} \times Pe_{j,\text{film}} + \text{ratio\_area\_tray} \times Pe_{j,\text{tray}} \times (1-\text{ratio\_area\_lid}) \)).

**c- Mass flow of gaseous species at the food sample interface**

The mass flow \( \varphi_{j,I} \) (kg s\(^{-1}\)) of gas species \( j \) (O\(_2\), CO\(_2\)) at the food sample interface is calculated according to:
\[ \varphi_{j,t} = k \frac{M_j A_I}{RT} (p_{j,HS,I} - p_{j,HS}) \]  

(5)

where \( k \) (m \( s^{-1} \)) is the external mass transfer coefficient at the interface between the food sample and the headspace assumed to be the same for \( O_2 \) and \( CO_2 \), \( A_I \) (m\(^2\)) the surface of this interface and \( p_{j,HS,I} \) (Pa) is the partial pressure of gas species \( j \) at the immediate vicinity of the food surface. Assuming the existence of a thermodynamic equilibrium for species \( j \) at the food surface, the concentration of dissolved gas species \( j \) at the food surface \( C_{j,F,x=0} \) (kg \( m^{-3} \)) is in relation with \( p_{j,HS,I} \) according to Henry’s law:

\[ p_{j,HS,I} = \frac{C_{j,F,x=0}}{M_j k_{H,j}} \]  

(6)

where \( k_{H,j} \) is the solubility coefficient of species \( j \) (mol Pa\(^{-1} \) m\(^3\)) in the food sample.

**d- Dissolved gas species diffusion within the food sample**

Diffusion of dissolved gaseous species within the food sample along the \( x \)-axis (Fig. 1) is described using Fick’s second law taking the form:

\[ \frac{\partial C_{j,F}}{\partial t} = D_j \frac{\partial^2 C_{j,F}}{\partial x^2} \]  

(7)

where \( C_{j,F} \) is the concentration of dissolved gas species \( j \) in the food sample (kg \( m^{-3} \)), \( D_j \) the apparent diffusivity of the species \( j \) in the food sample (m\(^2\) \( s^{-1} \)) and \( x \) (m) is the distance from the interface between food and headspace varying between 0 and \( e_F \) which is the thickness of food sample. The boundary condition written at the interface between the food sample and the headspace takes the form:

\[ D_j \frac{\partial C_{j,F}}{\partial x} = \frac{\varphi_{j,t}}{A_I} = k \frac{M_j}{RT} (p_{j,HS,I} - p_{j,HS}) \text{ at } x = 0, \forall t \]  

(8)

At the interface between the food sample and the tray, assuming that no flux occurs, the boundary condition takes the form:

\[ D_j \frac{\partial C_{j,F}}{\partial x} = 0 \text{ at } x = e_F, \forall t \]  

(9)
Assuming that the food sample was initially in equilibrium with a gas of fixed composition equal in terms of partial pressure to $p_{j,0}$ (Pa), the initial conditions take the form:

$$C_{j,F} = M_j k_{H,j} p_{j,0} \text{ at } t = 0, \forall x$$  \hspace{1cm} (10)

**e- Modelling the net production rate $S_{j,F}$**

The net production rate $S_{j,F}$ is due to microorganisms’ respiration that consumes $O_2$ and produces some $CO_2$. $S_{j,F}$ was modelled using the formalism of Mikaëlis-Menten as proposed in the work of Thiele et al. (2006).

$$S_{j,F} = \left( \frac{r_{O_2,max} p_{O_2,HS}}{K_m + p_{O_2,HS}} \right) \bar{N}_m$$  \hspace{1cm} (11)

Where $r_{O_2,max}$ is the maximum respiration rate (kg s$^{-1}$ CFU$^{-1}$), $K_m$ is the Michaelis-Menten constant (Pa), $p_{O_2,HS}$ (Pa) is the partial pressure of $O_2$ in headspace, $\bar{N}_m$ is the microorganism concentration (CFU g$^{-1}$) and $m$ is the mass of the food (g). It was assumed that the production of $CO_2$ was equal to the consumption of $O_2$ in the present study. $r_{O_2,max}$ and $K_m$ were estimated at 7°C from the work of Thiele et al. (2006) who modelled the respiration of *Pseudomonas fluorescens* using respiration experiments. $r_{O_2,max}$ value at 7°C has been used as a reference value in the Arrhenius law equation with an average activation energy of about 50 kJ mol$^{-1}$, value usually observed for respiration metabolism (Charles et al., 2005; Torrieri et al., 2009).

**f- Modelling microorganism growth**

The microbial growth was described by a logistic with delay growth model (Rosso, 1995; Rosso, Lobry, Bajard, & Flandrois, 1995).

$$\frac{dN_t}{dt} = 0 \text{ for } t \leq lag$$  \hspace{1cm} (12a)

$$\frac{dN_t}{dt} = \mu_{max} N_t \left( 1 - \frac{N_t}{N_{max}} \right) \text{ for } t > lag$$  \hspace{1cm} (12b)
where $N_t$ (CFU g$^{-1}$) is the value of the microorganism population at time $t$ and position $x$ within the food sample and $N_{\text{max}}$ (CFU g$^{-1}$) is the maximal population at the end of the growth curve (stationary phase), $\mu_{\text{max}}$ the maximal growth rate (s$^{-1}$) and $\text{lag}$ the lag time duration (h) for the microorganism of interest.

The effects of temperature, pH and water activity ($a_w$) on growth rate, were described following the gamma concept (Zwietering, Wijtzes, Wit, & Riet, 1992) associated to the cardinal models (Le Marc et al., 2002; Rosso et al., 1995). This semi-empirical model was chosen as the best compromise between simplicity of use and programming and because it includes some interpretable parameters (cardinal values).

\[ \mu_{\text{max}} = \mu_{\text{opt}} \gamma_T \gamma_{pH} \gamma_{a_w} \gamma_{O_2} \gamma_{CO_2} \xi \]  
(13)

where $\mu_{\text{opt}}$ (s$^{-1}$) is the optimal growth rate, $\gamma_W$ with $W = \{T, pH, a_w, O_2, CO_2\}$ are adimensional weighting parameters representing respectively the influences of environmental factors such as temperature, pH, water activity, dissolved $O_2$ and $CO_2$ concentrations over microorganism growth rate, $\xi$ being a function representing the interactions between the different environmental parameters.

$\gamma_T$, $\gamma_{pH}$ and $\gamma_{a_w}$ are calculated using cardinal models (Rosso et al., 1995) as detailed in the previous work of (Chaix et al., 2015a).

For MAP sensitive microorganisms, microbial growth equation is linked to $O_2/CO_2$ evolution in headspace (eq. 1) through two additional gamma functions in the secondary model (1) one for $CO_2$ (Eq. 14) and (2) one for $O_2$ (Eq. 16) as previously described by Guillard et al. (2016):

\[ \gamma_{CO_2}(x, T) = 1 - \frac{C_{CO_2,x}(x, t)}{C_{CO_2,\text{max}}} \]  
(14)

where $C_{CO_2,x}(x, t)$ is the concentration of dissolved $CO_2$ (kg m$^{-3}$) into the food sample at a given position $x$ and time $t$ and $C_{CO_2,\text{max}}$ is the maximal concentration of $CO_2$ (kg m$^{-3}$) withstanding by the microorganism (above this value, $\gamma_{CO_2}(x, t) = 0$ and no growth occurs). $C_{CO_2,\text{max}}$ is calculated from its equivalent in headspace in $\%$, $\%_{CO_2,\text{max}}$, as follows:
\[ C_{CO_2,max} = \%_{CO_2,max} p_T M_{CO_2} k_{H,CO_2} \]  

(15)

Where \( k_{H,CO_2} \) is the CO\(_2\) solubility coefficient (according to Henry’s law) in mol Pa\(^{-1}\) m\(^3\), \( M_{CO_2} \) is the molar mass of CO\(_2\) in kg mol\(^{-1}\), and \( p_T \) is the total pressure in Pa (usually the atmospheric pressure).

\[ \gamma_{O_2}(x, t) = \frac{C_{O_2,F}(x, t)}{C_{O_2,min} + C_{O_2,F}(x, t)} \]  

(16)

where \( C_{O_2,F}(x, t) \) is the concentration of dissolved O\(_2\) (kg m\(^{-3}\)) into the food sample at a given position \( x \) and time \( t \) and \( C_{O_2,min} \) (kg m\(^{-3}\)) is the minimal concentration required for microbial growth. \( C_{O_2,min} \) is calculated from the \( \%_{O_2,min} \) (%) as follows:

\[ C_{O_2,min} = \%_{O_2,min} p_T M_{O_2} k_{H,O_2} \]  

(17)

Where \( k_{H,O_2} \) is the O\(_2\) solubility coefficient (according to Henry’s law) in mol Pa\(^{-1}\) m\(^3\) and \( M_{O_2} \) is the molar mass of O\(_2\) in kg mol\(^{-1}\).

It appears from the above description (Eqs. 14 & 16) that \( C_{CO_2,max} \) and \( C_{O_2,min} \) are the two indispensable parameters for representing the effect of O\(_2\)/CO\(_2\) on microbial growth in the case of MAP sensitive microorganisms. Eqs. (14) and (16) are coupled to the system of partial differential equations (PDE) describing the evolution of O\(_2\)/CO\(_2\) concentrations within the food.

\( \xi \) in Eq. 13 describes the interactions between the environmental factors. \( \xi \) is calculated from interactions terms as described in Guillard et al., (2016).

In the present model, the determining factor in growth of gas-sensitive microorganisms, is the concentrations of dissolved O\(_2\)/CO\(_2\) at any point of the food, and especially at the food surface where growth generally occurs. This dynamic system leads to a challenging situation because the concentrations of the gases are a function of both time and space coordinates. In the field of predictive microbiology, the effect of a dynamic concentration of gas (CO\(_2\) and O\(_2\)) on microbial behaviour had never been considered except in our previous work (Chaix et al., 2015a; Guillard et al., 2016). The coupling of mass transfer models and predictive microbiology models requires working with a system...
of Partial Differential Equations (PDEs). The computer programme solved at any time and space point a set of coupled differential equations which represent for the present case-study the $O_2/CO_2$ concentration and microbial cells distribution profiles within the food. This had never been attempted before.

Independent input parameters are used to run the mathematical model. No model calibration is first required confirming the interest of semi-mechanistic models where input data are interpretable and could be determined using independent experiments or extrapolated from literature data. A summary of all input parameters required for running one simulation is given in Table 1. The model was previously validated using dedicated challenge-tests (Guillard et al., 2016) on poultry, processed cheese and salmon for *Pseudomonas fluorescens* and *Listeria monocytogenes* and was proved to adequately describe the experimental growth curves and $O_2$ and $CO_2$ evolutions with time without need of readjustment or parameter identifications.

2.3. Software development process of the MAP-OPT tool

The different steps of a software development time-line were followed, namely definition of requirements, programme design, coding, testing and software release.

2.3.1. Requirements

The requirements focus on satisfying the user's expectations regarding the software. The main requirement of MAP-OPT tool was to provide a predictive software tool allowing users to optimise packaging material and modified atmosphere of their fresh, non-respiring foods packed in MAP. It is based on the simulations of two interrelated phenomena: $O_2/CO_2$ evolution with time in the headspace and microbial growth. Coupling of the predictive software tool with data warehouse providing values for input parameters allows the user to test several types of food products, packed in various packaging materials (more than 300 materials currently stored in the data warehouse) and contaminated with a single bacteria among a list of microorganisms (two microorganisms currently available in the first prototype). In addition, the user has the possibility to easily explore and consult
the data warehouse using a dedicated application (@Web) that enables to find the material which would be the most suitable for his food product.

There are two ways to use the MAP-OPT tool depending on the user’s expectations (1) simple simulation mode or (2) decision making-mode which are described below and summarized in Fig. 4.

a) Simple simulation mode

In simulation mode (see Fig 4A), the user is able to simulate the impact of the packaging material or of the mixture of gases on the product safety, e.g. microbial growth. Type of microorganism, storage conditions and geometry of the system is set up by the user. It produces technical outputs such as microbial growth curve as a function of time of a given bacterial species, O2/CO2 permeation rate through the packaging material. The computer programme requires no less than 50 input parameters for each simulation. However, as previously stated (Chaix et al., 2015a), most of them are fixed (such as energy of activations which are expected to change in relatively narrow ranges) and only 11 parameters are finally relevant and asked for running a simulation. Fig. 5A shows the user interface in simple simulation mode with the scroll-down menu for selecting the composition of the tray. This scroll-down menu allows the O2/CO2/N2 permeabilities of the packaging material to be automatically retrieved from the @Web data warehouse. A second scroll-down menu exists for lid film selection, a third one for food selection and a fourth for microorganism selection. “Food” scroll-down menu allows solubility and diffusivity characteristics of the selected product to be retrieved from the corresponding data warehouse. “Microorganism” scroll-down menu allows all the required input parameters for predicting growth (e.g. cardinal values) to be implemented in the programme. All other input parameters, such as geometrical characteristics, duration and temperature of storage, initial headspace composition and initial microbial load, etc. are provided manually by the user. Outputs of this simulation mode are curves showing evolution of O2 and CO2 concentrations into headspace and corresponding microbial growth (Fig. 5B).

The user could also simulate the impact of microorganisms’ respiration on the evolution of headspace gases concentration in addition to phenomena of permeation through packaging and dissolution into the food.
b) Decision making-mode

Decision making-mode (see Fig 4B), is used in order to properly design the MAP system (e.g. chose the internal atmosphere composition, the right ratio of food volume to headspace volume) and to rationally select the packaging material using a requirement driven approach. Such approach starts from a constraint, i.e. the targeted maximal level of bacteria at the end of the shelf life. The MAP-OPT tool allows this constraint to be translated into target barrier properties for the packaging material required to maintain the protective atmosphere in a given range of tolerance throughout the shelf life. From these estimated permeability values the suitable packaging material is selected by querying the dedicated data warehouse via @Web application. The computational complexity is due to the fact that gas concentrations in the headspace are dependent on gas dissolution/diffusion within food, permeation through packaging materials and gas consumption/production by the naturally present microbiota. In such complex system, identification of the optimal gas permeabilities could be only achieved through virtual MAP simulations.

2.3.2. Design and programming

The MAP-OPT tool was implemented as a web application hosted on a dedicated platform (http://plasticnet.grignon.inra.fr/IateTools/).

The system of differential equations combining microbial and mass transfer equations of the semi-mechanistic model is solved using a dedicated algorithm “ode15s” developed in Matlab® computing software (The Mathworks Inc., Natick, Mass, USA) and adapted to stiff systems where each of the unknown variables may exhibit radically different variation kinetics. This algorithm adjusted automatically the size of the time step used for numerical integration of the equations.

The data warehouse is based on W3C recommended knowledge representation languages (OWL and RDF) and could be filled in, examined and queried using a dedicated application @Web based on W3C SPARQL language, hosted on the same web platform.

The user-friendly interface is a web application, IateTools, developed in C#, under the Visual Studio integrated development environment from Microsoft. MATLAB toolboxes (DotNetBuilder, Compiler) allow to package MATLAB programmes as .NET assemblies which are easy to use by .NET
application like IateTools. So, users can run simulations royalty free even if they don’t have MATLAB licences. IateTools couple data warehouse information (food, package, microbial and environment parameters) to perform the simulations.

From the interface, the user selects the food, microorganism, packaging materials, gas composition and temperature. These parameters, once put in the model, e.g. MATLAB files, which are running on the server side, allow to run the simulation. Outputs are curves with the evolution of O₂ and CO₂ concentrations into headspace and corresponding microbial growth (Fig. 5B).

2.3.3. Testing

The software was tested by executing predefined scenarios with known results (e.g. challenge-tests that were specifically carried out to validate the mechanistic model coupling mass transfer & microbial growth (Guillard et al., 2016). MAP-OPT tool was tested and validated in isothermal condition at 4, 8 and 15°C. If deviations were noticed, they were sent back to coding for corrections followed by a new test round.

Database concerning bacteria is actually limited because the effect of O₂ and CO₂ on microbial growth is scarcely modelled, and therefore $C_{CO_2,max}$ and $C_{O_2,min}$ parameters are often lacking. At the moment, a set of complete cardinal values including effect of O₂ and CO₂ gases on growth is available only for two microorganisms (Listeria monocytogenes and Pseudomonas fluorescens). The MAP-OPT tool was validated for these two microorganisms.

The food database is also restrictive to four real food products, exclusively products for which the values of O₂ and CO₂ diffusivity and solubility are known. The lack of values concerning these two parameters is less restrictive for the MAP-OPT tool than the lack of microorganism data. Indeed, sensitivity analysis has revealed that model simulations were not sensitive to the value of diffusivity and solubility describing diffusion of gases into the food product. Therefore, by selecting for instance, poultry meat in the scroll-down menu of the MAP-OPT software, the user could simulate the behaviour of many other meat products with very limited error on gas diffusion.
2.3.4. Current limitations of the MAP-OPT tool

With the present on-line prototype, only isothermal conditions could be tested but further releases should include temperature cycles and the possibility for the user to upload his own file (.txt, .csv, .xls, etc.) of temperature variations. The raw programme file already includes this possibility. With the current software release, it is not possible for the user to define properties of a material not included in the drop-down list. It should be possible in future releases.

The present MAP-OPT prototype does not yet include stochastic module in order to test the variability of bacterial strain, of O$_2$ consumption by aerobes and more generally biological variability inherent to any living system. This will be addressed in an up-graded version. Like most traditional tools of predictive microbiology, only one unique bacteria strain is considered per simulation while in practice a consortium of bacteria simultaneously grows and interacts with each other. Improvement of this last point is definitively dependent on how the microbiologists will address this issue in the near future to significantly improve the relevance of predictive microbiology modelling. A special effort should be made also to quantify the effect of gases (O$_2$ and CO$_2$) on a large panel of gas-sensitive microorganisms and the metabolism of aerobes.

As a consequence of these limitations, the MAP-OPT software could not be used at the moment as a tool for regular safety assessment. However, in a context of transition toward circular economy and food waste and losses reduction, MAP-OPT software is an asset for helping the user to design his MAP system in a more sustainable way, simulating the impact on food preservation of innovative food packaging technologies, e.g. monolayer, easy to recycle or bio-based & biodegradable packaging materials.

3. Availability of the MAP-OPT tool

A free demo version of the MAP-OPT tool is available on the INRA web platform named Plastic, at http://plasticnet.grignon.inra.fr/IateTools/MapOpt. It is a version limited to the functionalities of the simulation mode in isotherm condition: it allows to test the impact on microbial growth of different packaging materials among those stored in the data warehouse and different gas compositions. Only
three different foods (salmon, cheese and poultry meat) and two microorganisms (*Pseudomonas fluorescens* and *Listeria monocytogens*) are available at the moment. Characteristics of the system could be defined by the user or, if needed, could be uploaded from previous data set. The user could use his own optimal growth rate adapted to his product. Results of the current simulation could be saved for further comparison. Using this free demo, the user will be able to appreciate the impact on microbial growth of his own choice of packaging and/or atmosphere. A free login could be created upon request to the administrator to benefit of all functionalities.

A free demo of the @Web application is available at [http://pfl.grignon.inra.fr/atWeb/](http://pfl.grignon.inra.fr/atWeb/) and allows the user to explore the data stored in the data warehouse and to make some queries.

### 4. MAP-OPT tool for decision making use-cases

In order to illustrate the strategy of decision-making facilitated by the use of the MAP-OPT software, we now consider a case study, poultry meat stored at 8°C in MAP. The target microorganism to control is *Pseudomonas fluorescens*, a strict aerobe requiring O₂ to grow, and inhibited by CO₂. The questions are which atmosphere composition and packaging material for the lid film must be used to limit the growth of *Pseudomonas* on meat in given conditions (fixed mass of food and packaging geometry)? The dimensions of the system were imposed by the tray sealer dimensions and the mass of the food per pack (about 400 g). It was found that trays in PS/EVOH/PE of about 10x15x5 cm³, i.e. a total volume of exactly 732 mL (directly measured on commercial trays) were adapted to pack 400 g of poultry meat. These trays were chosen as container. Given the thickness of the tray (0.65 mm), thick as compared to the lid film (0.055 mm), and its very low permeability (PO₂= 2.62x10⁻¹⁹ and PCO₂= 1.57x10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹), we considered in first hypothesis that the mass transfer through the sides of the tray is negligible: only the permeation through the lid film, i.e. through a surface of 209 cm², would contribute to internal atmosphere changes.

In these conditions, we wanted to determine which type of lid film material should be used to maintain the modified atmosphere in such a way that microorganism growth remains below a threshold value fixed at 4 log CFU/g.
The mass of food measured on tens of poultry pieces was about 410 g. All other criteria (solubilities, diffusivities, microbial parameters) were retrieved from the data warehouse and are summarized in the Supplementary material (S1). We considered an initial contamination of 10 CFU / g (corresponding to the inoculum that is deposited on the surface of the meat previously ionised 7.5 kGy using Aerial facilities to inhibit the development of naturally present microflora).

Preliminary simulations made by the MAP-OPT software have revealed that, in the conditions described above of pack geometry and mass of food selected for this case study, a headspace composition of about 50% CO₂ and 50% N₂ would be suitable to prevent *P. fluorescens* growth below 4 log CFU/g at the use-by-date (a theoretical value of 15 d was chosen for demonstration purpose). Furthermore, we know that industrial facilities do not allow all O₂ in headspace to be removed during gas flushing and that about 1-2% of O₂ still remain in the pack. Therefore, the initial internal gas composition to consider in this case study is 50% CO₂, 2% O₂ and 48% N₂.

The MAP-OPT tool was then used to test some values of O₂ and CO₂ permeabilities and to identify some couples of suitable values for this application (Fig. 6). The Matlab code was used instead of web application to be able to directly change the value of the permeability (functionality not yet available on the on-line release). The microorganism’s respiration was supposed to significantly consume O₂ and produce CO₂, therefore, the respiration option was set up.

Several decreasing permeability values were successively tested, from 1×10⁻¹⁵ to 1×10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹ for O₂ permeability (PO2) and from 5×10⁻¹⁵ to 5×10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹ for CO₂ permeability (PCO2). The max values correspond approximately to LDPE-based material, i.e. material displaying low gas barrier properties. The min values would correspond to a material with high barrier properties. We kept the ratio of PCO2 to PO2 (about 5) constant, as it is the ratio usually observed for conventional oil-based packaging materials. Fig. 6 shows that PO2 of 1×10⁻¹⁵ and 1×10⁻¹⁶ Pa⁻¹ mol m⁻¹ s⁻¹ Pa⁻¹ and corresponding PCO2 of 5×10⁻¹⁵ and 5×10⁻¹⁶ Pa⁻¹ mol m⁻¹ s⁻¹ Pa⁻¹ are not sufficient to maintain microbial growth below the threshold value of 4 log CFU/g while all values of PO2 below or equal to 1×10⁻¹⁷ Pa⁻¹ mol m⁻¹ s⁻¹ Pa⁻¹ and PCO2 below and equal to 5×10⁻¹⁷ Pa⁻¹ mol m⁻¹ s⁻¹ Pa⁻¹ are suitable.
The Pseudomonas growth in such MAP systems is complex and results in both effects: CO₂ inhibition at the beginning and lack of O₂ at the end of the simulation. The initial quantity of CO₂ in headspace is sufficient to inhibit microbial growth on the food surface. However, this CO₂ content decreases due to CO₂ dissolution in the food and CO₂ permeation toward external atmosphere. When CO₂ drops below 30% (as it is the case for the material with high permeability, e.g. PCO₂=5×10⁻¹⁵ mol m⁻¹ s⁻¹ Pa⁻¹), its quantity in headspace and dissolved in food is not sufficient anymore to significantly inhibit Pseudomonas growth. In this system, Pseudomonas growth could occur because of the residual O₂ amount (about 2%). Due to Pseudomonas respiration, the amount of residual O₂ is consumed in the headspace stopping the growth when the O₂ level drops below 0.25% as noticed in previous work (Guillard et al., 2016). The O₂ consumption substitutes for the inhibiting effect of CO₂ in the present case study leading to a sudden stop in the simulated growth curve (and a plateau as seen in Fig. 6).

When the two lower barrier films are used, the inhibiting effect of CO₂ is lost too quickly to be compensated by the disappearance of O₂ therefore, growth is much greater. Following the results of Fig. 6, no difference is obvious between this microbial curve obtained with a PO₂=1×10⁻¹⁸ mol m⁻¹ s⁻¹ and PCO₂=5×10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹ and the one corresponding to PO₂=1×10⁻¹⁷ mol m⁻¹ s⁻¹ Pa⁻¹ and PCO₂=5×10⁻¹⁷ mol m⁻¹ s⁻¹ Pa⁻¹. There is a threshold of PO₂ and PCO₂ below which there is no more effect on the shape of the microbial curve because CO₂ and O₂ contents inside the pack remain high enough and close enough to 0 respectively to completely inhibit the Pseudomonas growth. Both materials could have been equally selected but, considering a safety margin, we chose the one with the lowest permeabilities, PO₂=1×10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹ and PCO₂=5×10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹.

In view of the variation in gas permeability values for the candidate materials ultimately identified for the lid film, the hypothesis of negligible transfer through the tray sides has been then tested. Considering both extreme values of PO₂ for the lid film (1×10⁻¹⁵ and 1×10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹), two simulations were conducted (1) one considering the lid film only and (2) one considering the lid film and the tray sides in the mass transfer calculations. In the case of the value of O₂ permeability 1×10⁻¹⁸ mol m⁻¹ s⁻¹ Pa⁻¹ for the lid, the differences between the two conditions tested were found to be negligible. Therefore, in the conditions tested here (surface and volume of package, mass of food,
simulation time), the hypothesis of neglecting mass transfer through the tray sides seems justified (Fig. 7).

The second step of our decision-making strategy is to find the packaging materials displaying such values of permeabilities. This could be done by querying our packaging data warehouse, which contains nowadays more than 350 permeability values. The @Web application was used to build the query Fig. 8A and find the ranking of the most suitable packaging as shown in Fig. 8B. In the current release, queries in @Web must be done one by one. Therefore, even if O₂ and CO₂ permeabilities should be met at the same time, we worked on O₂ permeability only, first. Then we try to check if PCO₂ also matches, which should be the case because a selectivity of around 5 between PO₂ and PCO₂ has been used in our simulations, which applies for most commercial oil-based materials.

In our case study, the query made on O₂ permeability value gave more than 5 materials as answers, one being ranked in first position. Thanks to the query’s results, the most suitable material (rank 1) would be a multilayer made of OPET/EVOH/PE. Let us notice that reliability indicators associated with this material reveal a contradiction between metadata (denoted in Fig. 8B by the icon in the Reliability score column) which can be explained in Fig. 2: the criterion Source type has a high quotation regarding the reliability in order to take into account that the document benefited from an external peer-review and the Criterion Repetition has a low quotation as no repetition value which means that annotated experimental data don’t provide any information about their variability. As CO₂ permeability of the packaging of rank 1 was also annotated in this document with the value $5.24 \times 10^{-18}$ mol/m/s/Pa, it is possible to check if this material also fits the CO₂ permeability requirement. Material of rank 2 would be a polyimide.

The last step consists in testing these materials selected for a final validation. This was done through dedicated challenge tests realized following the procedure presented in (Guillard et al., 2016). Material of rank 1 was used to seal a tray and carry out a challenge test at 8°C with poultry meat initially inoculated with $10^1$ CFU/g. PO₂ and PCO₂ of this material (OPET/EVOH/PE), taken from the data warehouse, are $1.04 \times 10^{18}$ Pa⁻¹ mol m⁻¹ s⁻¹ Pa⁻¹ and $5.24 \times 10^{18}$ Pa⁻¹ mol m⁻¹ s⁻¹ Pa⁻¹ respectively. All other experimental conditions (e.g. geometry of the tray and lid film, mass of food, etc.) were kept as
in the preliminary simulations used for identifying suitable PO2 and PCO2. All parameters are gathered in Table 1.

Comparison between experimental and predicted technical outputs made by the simulation programme are shown in Fig. 9. In the present case, O₂ and CO₂ in headspace and microbial cell count are relevant technical outputs because there are also the easiest accessible by experiment. Comparison between experimental and technical outputs reveals some discrepancies: the plateau observed on the theoretical growth curve is not well observed on the experimental curve and O₂ concentration in headspace is globally over- and underestimated by the model. Discrepancies principally occur due to the fact that our model predicts that no more O₂ remains in the package after 5 days while experimentally there is always close to 0.20-0.30% of residual O₂ which is enough to sustain *Pseudomonas* growth. Thus, *Pseudomonas* is, by the model, more strongly affected by the O₂ content than in reality.

Moreover, the dynamic of O₂ in the headspace is not also well predicted: the peak of O₂ after a few days of storage is much more marked in theory than in practice. This could be explained by two concomitantly phenomena that could have antagonistic effect: (1) the model for O₂ consumption could not represent the reality of O₂ consumption by the microorganisms in the package well and (2) a leak in the package could occur with O₂ continuously coming in the package that partially compensates the consumption (therefore, a residual O₂ concentration is still observed). Moreover, the minimal O₂ content necessary for *Pseudomonas* growth may be not strictly at 0.25% as stated in the model and would gain to be a more fine-tuned control.

In addition to the present work, it must be noted that more than 10 experimental challenge tests (see Guillard et al. 2016, Chaix et al. 2015b) have been conducted and have allowed to validate the model for two types of microorganisms, three types of food and packaging, three temperatures and two different atmosphere conditions. Therefore, considering the complexity of the underlying mathematical model, the numerous experimental validations conducted and in spite of biological variability and parameters uncertainty that is not computed in this first prototype, we can consider that predictions of the MAP-OPT tool relatively well matched the experimental results. Even if discrepancies occur, it is enough to conclude about MAPT-OPT tool validity and to stress all its potential applications.
6. CONCLUSION

In this paper, we have proposed the MAP-OPT software, a modelling tool able to predict microbial growth and gas mass transfer in a packed food coupled with a data warehouse of food and packaging characteristics for a better decision process and a shortened optimisation step of the MAP system. This software was proved to be efficient to help the user in the design of his MAP system. The case-study provided here on poultry meat illustrated well how this tool could be used to find the packaging material suitable for a given product in a given set of storage conditions. The MAP-OPT tool could also be used by several stakeholders of the food chain for numerical exploration, to test different storage conditions, gas composition or packaging materials. An effort must be made in the future on the updating of the existing data warehouse, gathering packaging, food and microbial parameters in order to improve the decision support issues. In addition, the effect of different humidity conditions is not yet included in the model proposed while water vapour transfer in the system could significantly affect packaging gas permeability especially in the case of water sensitive materials. This should be addressed in further release of the software.
7. SYMBOLS, ACRONYMS

\( A \) Surface

\( C \) Mass concentration (within gas or condensed phase)

\( C_{CO_2, max} \) maximal concentration of CO\(_2\) (kg/m\(^3\)) withstanding by the microorganism (above this value, no growth occurs)

\( C_{O_2, min} \) minimal concentration required for microbial growth (kg/m\(^3\)).

\( C_{j,F} \) concentration of dissolved gas species \( j \) (O\(_2\), CO\(_2\)) into the food sample (kg/m\(^3\))

\( C_{j,HS} \) concentration of gas species \( j \) (O\(_2\), CO\(_2\) and N\(_2\)) in the headspace (kg/m\(^3\))

\( D \) Apparent diffusivity

\( DST \) Decision Support Tool

\( e \) Thickness

\( E_a \) Activation energy in Arrhenius law

\( Lag \) Lag time for microbial growth

\( LDPE \) low density polyethylene

\( k_H \) Solubility coefficient (according to Henry’s law)

\( M \) Molar mass

\( MAP \) Modified Atmosphere Packaging

\( N \) Microorganism population

\( OPET/EVOH/PE \) oriented polyethylene terephthalate/ ethylene vinyl-alcohol/polyethylene

\( OWL \) Web Ontology Language

\( p \) Partial pressure

\( PCO_2 \) carbon dioxide permeability

\( Pe \) Permeability of a gas species through the lid film

\( PO_2 \) oxygen permeability

\( PS/EVOH/PS \) polystyrene/ethylene vinyl-alcohol/ polystyrene

\( P_f \) Total pressure in the headspace (assumed constant)

\( R \) Ideal gas constant
RDF Resource Description Framework

$S$ Net mass production rate of gas species by microbial activity

SPARQL SPARQL Protocol and RDF Query Language

$T$ Temperature

$T$ Time

$V$ Volume

W3C World wide web consortium (https://www.w3.org/)

$x$ Spatial coordinate

Greek letters

$\gamma$ Adimensional weighing parameter representing the influence of environmental parameters over microbial growth rate

$\mu$ Growth rate for microbial growth

$\xi$ Adimensional weighing parameter representing the influence of the interactions between environmental parameters over microbial growth rate

$\phi$ Mass flow

Subscripts, superscripts

$\infty$ Relative to the surrounding atmosphere

$F$ Food sample within the food/packaging system

$HS$ Headspace volume within the food/packaging system

$I$ Interface between headspace volume and food or in the headspace at the immediate vicinity of the food surface (for equilibrium partial pressure calculation)

$J$ Gas species: $O_2$, $CO_2$ or $N_2$

$L$ Lid film

$max$ Maximum

$min$ Minimal

$Opt$ Optimal
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 Figures caption

Figure 1: An example of ontological conceptual modelling: the O\textsubscript{2} permeability relation concept

Figure 2: Expert judgement quotations associated with the metadata “Source type” (A) and reliability assessment of a document using metadata (B)

Figure 3: Scheme describing the system tray + lid film used in the modelling approach. Main biological and physical mechanisms modelled are indicated on this figure

Figure 4: The software design of the MAP’OPT tool (A) simulation mode and (B) decision making mode

Figure 5: (A) Main window of the user-friendly interface for the MAP-OPT tool, showing the scroll-down menu for selecting the tray material and (B) example of model outputs for chicken stored at 6°C and contaminated by Pseudomonas fluorescens

Figure 6: Impact of decreasing values of O\textsubscript{2} and CO\textsubscript{2} permeabilities on O\textsubscript{2} and CO\textsubscript{2} concentration in headspace and P. fluorescens growth evolution as a function of time (8°C on poultry meat). Permeabilities are given at 20°C and are recalculated in the programme at 8°C using Arrhenius law.

Figure 7: Simulations comparing two hypotheses of modelling, (1) mass transfer occurs through the lid film (solid lines) only and (2) mass transfer occurs through the lid film + tray sides (dotted lines), for two different values of O2 and CO2 permeability for the lid film: PO2= 1x10\textsuperscript{-15} and PCO2= 5x10\textsuperscript{-15} mol m\textsuperscript{-1} s\textsuperscript{-1} Pa\textsuperscript{-1} (Fig. 6A) and PO2= 1x10\textsuperscript{-18} and PCO2= 5x10\textsuperscript{-18} mol m\textsuperscript{-1} s\textsuperscript{-1} Pa\textsuperscript{-1} (Fig. 6B). Dotted and solid lines are overlapped on Fig. 6B.

Figure 8: Query of the data warehouse using @Web module: query building (A) and results of the query (B)

Figure 9: Evolution as a function of time of O\textsubscript{2} and CO\textsubscript{2} headspace concentration and Pseudomonas fluorescens growth on poultry meat surface, stored at 8°C during 16 d in MAP (50% initial CO\textsubscript{2} / 50% initial N\textsubscript{2}). Symbols are experimental data and solid lines simulations.
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Figure 5: (A) Main window of the user-friendly interface for the MAP-OPT tool, showing the scroll-down menu for selecting the tray material and (B) example of model outputs for chicken stored at 6°C and contaminated by *Pseudomonas fluorescens*
Figure 6: Impact of decreasing values of O\textsubscript{2} and CO\textsubscript{2} permeabilities on O\textsubscript{2} and CO\textsubscript{2} concentration in headspace and \textit{P. fluorescens} growth evolution as a function of time (8°C on poultry meat). Permeabilities are given at 20°C and are recalculated in the programme at 8°C using Arrhenius law.
Figure 7: Simulations comparing two hypothesis of modelling, (1) mass transfer occurs through the lid film (solid lines) only and (2) mass transfer occurs through the lid film + tray sides (dotted lines), for two different values of O$_2$ and CO$_2$ permeability for the lid film: PO$_2$= 1x10$^{-15}$ and PCO$_2$= 5x10$^{-15}$ mol m$^{-1}$ s$^{-1}$ Pa$^{-1}$ (Fig. 6A) and PO$_2$= 1x10$^{-18}$ and PCO$_2$= 5x10$^{-18}$ mol m$^{-1}$ s$^{-1}$ Pa$^{-1}$ (Fig. 6B). Dotted and solid lines are overlapped on Fig. 6B.
Figure 8: Query of the data warehouse using @Web module: query building (A) and results of the query (B)
Figure 9: Evolution as a function of time of $O_2$ and $CO_2$ headspace concentration and *Pseudomonas fluorescens* growth on poultry meat surface, stored at 8°C during 16 d in MAP (50% initial $CO_2$ / 50% initial $N_2$). Symbols are experimental data and solid lines simulations.
Table 1: Input parameters used in the MAP-OPT program file for the studied case study. All data from Guillard et al. (2016), unless otherwise specified.

<table>
<thead>
<tr>
<th>PARAMETER</th>
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<td><strong>Food characteristics</strong></td>
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<td>Food mass</td>
<td>(g)</td>
<td>m</td>
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<tr>
<td>Food pH</td>
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<td>5.62 **</td>
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<tr>
<td>Food $a_w$</td>
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<td><strong>Packaging characteristics</strong></td>
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<tr>
<td>Film thickness</td>
<td>(m)</td>
<td>$e_L$</td>
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<tr>
<td>Film area</td>
<td>(m²)</td>
<td>$A_L$</td>
<td>2.09 x10^{-2} *</td>
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<tr>
<td>Film thickness</td>
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<td>Total volume packaging</td>
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<td>$V$</td>
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<tr>
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<td>Tray dimension</td>
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<td>20.0 x 3.5 x 10^{-5}</td>
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<tr>
<td><strong>Gas permeabilites and activation energies</strong></td>
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<tr>
<td>Film O₂ permeability (at 23°C)</td>
<td>(mol/m.s.Pa)</td>
<td>$P_{eO_2}$,(film)</td>
<td>1.04×10^{-18}</td>
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<td>Film CO₂ permeability (at 23°C)</td>
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<td>Film N₂ permeability (at 23°C)</td>
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<tr>
<td>Tray O₂ permeability (at 23°C)</td>
<td>(mol/m.s.Pa)</td>
<td>$P_{eO_2}$,(tray)</td>
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<tr>
<td>Tray CO₂ permeability (at 23°C)</td>
<td>(mol/m.s.Pa)</td>
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<td>Tray N₂ permeability (at 23°C)</td>
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<td><strong>Gas permeabilites and activation energies</strong></td>
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<td>O₂ solubility coefficient (at 20°C)</td>
<td>(mol/kg.Pa)</td>
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<td>CO₂ solubility coefficient (at 4°C)</td>
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<td>O₂ diffusivity coefficient (20°C)</td>
<td>(m²/s)</td>
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<td>CO₂ diffusivity coefficient (20°C)</td>
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<td>External mass transfer coefficient at HS/F interface</td>
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<td><strong>Initial conditions</strong></td>
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<td>Surrounding atm. total pressure</td>
<td>(Pa)</td>
<td>$P_T$</td>
<td>1.01×10^{5}</td>
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<td>SYMBOL</td>
<td>VALUE</td>
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<td>Surrounding atm. O(_2) partial pressure</td>
<td>(%)</td>
<td>(p_{O_2,\infty})</td>
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<td>Surrounding atm. CO(_2) partial pressure</td>
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<td>(p_{CO_2,\infty})</td>
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<td>Surrounding atm. N(_2) partial pressure</td>
<td>(%)</td>
<td>(p_{N_2,\infty})</td>
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<tr>
<td>Headspace O(_2) partial pressure</td>
<td>(%)</td>
<td>(p_{O_2,HS})</td>
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<tr>
<td>Headspace CO(_2) partial pressure</td>
<td>(%)</td>
<td>(p_{CO_2,HS})</td>
<td>50 *</td>
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<tr>
<td>Headspace N(_2) partial pressure</td>
<td>(%)</td>
<td>(p_{N_2,HS})</td>
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<tr>
<td>Molar mass of O(_2)</td>
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<td>(M_{O_2})</td>
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<td>kg/mole</td>
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<td>Molar mass of N(_2)</td>
<td>kg/mole</td>
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<tr>
<td>Perfect gas constant</td>
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### Microbial growth parameters

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<th>Unit</th>
<th>Value</th>
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<tr>
<td>Initial bacteria concentration</td>
<td>(CFU/g)</td>
<td>(N_0) 6.02 – 23.98 *</td>
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<td>Maximal bacteria concentration</td>
<td>(CFU/g)</td>
<td>(N_{\text{max}}) 10(^{8.8})</td>
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<td>Lag time</td>
<td>(s)</td>
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<tr>
<td>Optimal growth rate</td>
<td>(h(^{-1}))</td>
<td>(\mu_{\text{opt}}) 2.88</td>
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<td>(°C)</td>
<td>(T_{\text{min}}) -7.36</td>
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<tr>
<td>Optimal temperature for growth</td>
<td>(°C)</td>
<td>(T_{\text{opt}}) 29.92</td>
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<tr>
<td>Maximal temperature for growth</td>
<td>(°C)</td>
<td>(T_{\text{max}}) 30</td>
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<tr>
<td>Minimal pH for growth</td>
<td></td>
<td>(pH_{\text{min}})</td>
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<td>Optimal pH for growth</td>
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<td>(pH_{\text{opt}}) 6.21</td>
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<td>Maximal pH for growth</td>
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<td>(pH_{\text{max}}) 2(\ast)(pH_{\text{opt}}) - (pH_{\text{min}})</td>
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<td>Minimal (a_w) for growth</td>
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<td>(a_{\text{wmin}}) 0.957</td>
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<tr>
<td>Optimal (a_w) for growth</td>
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<td>(a_{\text{wopt}}) 0.997</td>
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<td>Maximal CO(_2) concentration for growth (Headspace)</td>
<td>(%)</td>
<td>(%_{CO_2,\text{max}}) 40</td>
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<tr>
<td>Minimal O(_2) concentration for growth</td>
<td>(%)</td>
<td>(%_{O_2,\text{min}}) 0.25</td>
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</table>

### Respiration of microorganisms

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximal respiration rate at 7°C</td>
<td>kg/CFU.s</td>
<td>(r_{O_2,\text{max}}) 6.13x10(^{-18}) ****</td>
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<tr>
<td>Activation energy of (r_{O_2,\text{max}})</td>
<td>kJ/mole</td>
<td>(E_{a,r_{O_2,\text{max}}}) 50 ****</td>
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<tr>
<td>Mickaëlis-Menten constant</td>
<td>Pa</td>
<td>(K_m) 4571.6 ****</td>
</tr>
</tbody>
</table>

\*this study

** max. standard deviations for temperature, pH and \(a_{w}\) are ±0.8, ± 0.02 and ± 0.004 respectively. At least 3 replications.

*** kindly provided by LNE

**** from Thieie et al. (2006)

***** from Charles et al. (2005), Torrieri et al. (2009)