PredOxyPack® : How to predict the impact of the cold chain conditions on the oxygen barrier properties of packaging

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Introduction

Modified atmosphere packaging (MAP), including vacuum packaging, is a well-known technique used to prolong the shelf life of perishable food products. By eliminating or replacing the air surrounding a packed food product, various deteriorative processes that occur in food can be restricted mostly by reducing O_2-concentrations and increasing CO_2-concentrations. As it is important to maintain the modified atmosphere in the packaging during the shelf life of the product, there has been an increased interest in the production of different packaging concepts. The O_2-concentration in the packaging is thereby determined by (*i*) the residual O_2 after packaging which is dependent on the filling-system and (*ii*) the O_2 ingress during the shelf-life. To prevent this O_2 ingress, different barrier packaging materials can be used. The permeability of these packaging material is dependent on the polymer type, temperature, relative humidity, nature of the polymer (e.g. crystallinity, orientation, etc.), thickness of the polymer and differences in partial pressure of the gasses. Next to the O_2 barrier, the packaging should also have a good water vapor barrier, good mechanical strength and low cost. As there is no polymer which has all these features, multilayers are often used. This implies that there exists a multitude of packaging materials for different conditions which makes it very difficult for the user to choose the right packaging material. Besides, on the technical sheets the permeability's are often mentioned at 20-25°C while a lot of packed food products are stored in the cold chain. Therefore it is difficult to estimate the permeability of the packaging configuration under realistic storage conditions. To fill these gaps the software PredOxyPack® (www.predoxypack.com) has been developed in collaboration with Food2Know based on previous results of a Flanders' FOOD project.

Methodology

Permeation of gas through a polymer packaging material is characterized by a sorption-diffusion-desorption mechanism (Fig.1). The transfer of the molecules is driven by the difference in partial pressure across the film. Therefore the permeability coefficient *P* (ml O_2 . µm/m² . d . atm) can be calculated by Eq.1

$$P = \frac{Q\ .\ L}{A\ .\ t\ .\ \Delta p} \qquad \text{Eq. 1}$$

with Q the amount of permeant (ml O_2), diffusing through a polymer surface A (m²) over a period of time *t* (d), for *L* the thickness of the film (µm) and for Δ*p* a difference in partial pressure between the inner and outer atmosphere (atm) (Robertson, 2006). This permeability coefficient is often substituted on technical sheets by the OTR (Oxygen Transfer Rate, (ml O_2/m² . d . atm)) which is independent on the thickness of the film.

The permeability characteristics of polymeric materials are temperature dependent. For the major polymeric materials, this temperature dependency, as given by the activation energy of the permeability process, Ep, is included in the software, enabling to consider the impact of temperature changes upon the permeability.

For multilayer packaging materials the overall permeability is calculated based on the thickness of the total structure and the individual thicknesses and permeability's of the individual layers (Van Bree et al., 2010). In this formula, only consecutive layers are considered and the possible influence of adhesives is excluded.

Using these fundamentals of the permeation process, PredOxyPack® was developed, allowing to predict the dynamics of the oxygen concentration within the headspace of a packaging as a function of time for a selection packaging design throughout a dynamic temperature regime.

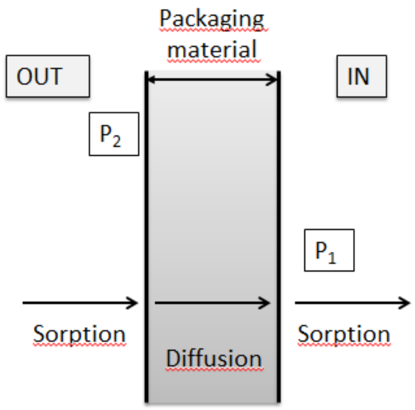

Fig. 1: Permeability model for gas transport throughout a polymer packaging material (adapted from: Robertson, 2006). P_1 and P_2: partial pressure of the permeating component at respectively the inner and outer side of the packaging material

Validation of the model

The validation of the model was performed for monolayer and multilayer films and for the combination of bottles and caps, taking into account different temperatures. This validation is thoroughly discussed in Van Bree et al. (2010). To quantify the performance of the simulation software, the observed and predicted O_2 concentrations were used to determine the R^2, the bias (B_f) and accuracy factor (A_f). In general the R^2 was high for the films (> 99.3%), indicating a good fit. Nevertheless, the A_f and B_f showed a slight underestimation for the majority of the data points. Moreover, the predictions for the multilayer were a little bit worse than the monolayer. This can be explained by the deviation of the permeability's of the individual layers, the non-uniformity of the thickness of the layers and the use of adhesives. For bottle and caps the R^2 was 0.86. Contrary to the films, the bias factor indicated a small overestimation

Description of the software

PredOxyPack® allows the user to predict the oxygen ingress for different packaging configuration, materials and time-temperature profiles. In this way realistic estimations can be made for the circumstances to which the food is exposed during its preservation including cold chain conditions. For the development of PredOxyPack® a lot of attention is paid to the user-friendliness by among others (*i*) the incorporation of predefined packaging configuration (Fig. 2) for which the exchange surfaces and volumes are automatically calculated, (*ii*) the automatic unit conversions and (*iii*) a build-in permeability database of different packaging materials with minimum, maximum and default values of OTR's.

Next to the predefined packages, the user can also choose a custom package consisting of one or two different packaging materials (Fig. 2). A bag consist always out of one material (mono- or multilayer), while for a tray and a bottle the distinction can be made between the body and the topfoil or the bottle and the cap, respectively. For the cylinder the user can choose different materials for body, top and bottom.

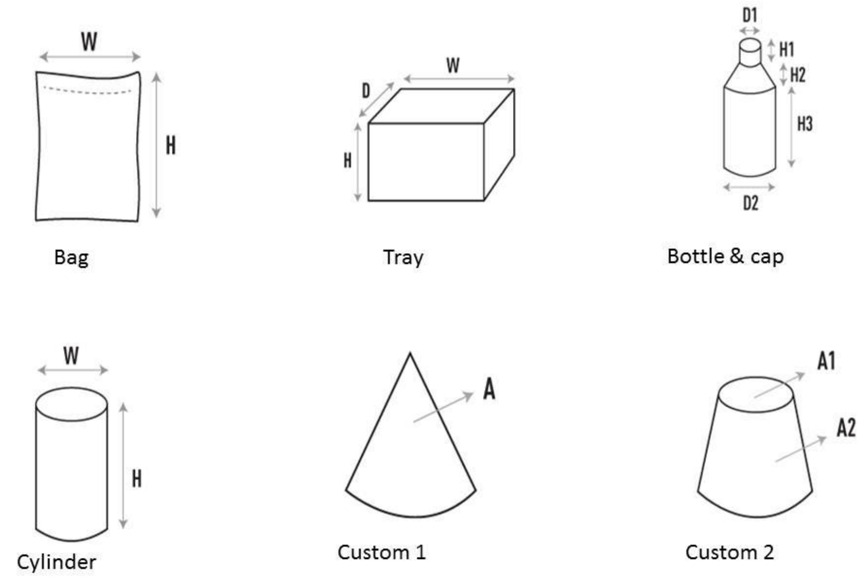

Fig. 2: Overview of the different packaging configuration incorporated in PredOxyPack®

Once the user has chosen the packaging configuration, the composition of the packaging material can be inserted for each packaging component separately (Fig. 3). The software allows easily to insert or delete an extra layer. Next to the polymer type, the user has to indicate the OTR, test thickness and test temperature of the polymer. These data can be either filled in by the user based on technical sheets or automatically appear in the software based on a build-in database with default values for each polymer type. Finally the user has to fill in the actual layer thickness of the polymer in the multilayer. Based on this information, the residual O_2 level after filling and the time temperature profile to which the packed product is exposed during filling, transport and storage, the oxygen evolution in the package can be calculated.

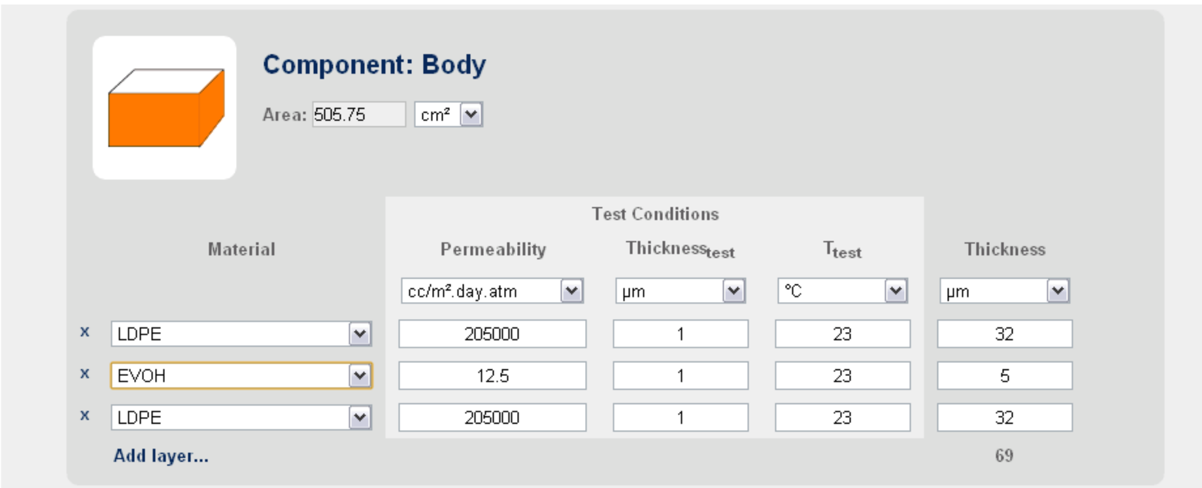

Fig. 3: Variables of the individual layers in a multilayer packaging

The output screen of the software (Fig. 4 and 5) represents a graphical output of the simulations (% or ppm O_2 in the headspace as a function of time) together with the followed temperature profile. Next to this graph, a table with the summary of the input values is mentioned. This is important when a user wants to reopen previous performed simulations.

Users of PredOxyPack®

PredOxyPack® is used by among others food business operators, converters, packaging designers. It can help Food Business Operators (FBO) to make the translation from the O_2 permeability which is mentioned on a technical sheet towards their specific packaged product during the reasonable foreseen conditions of storage e.g. within the cold chain. PredOxyPack® can give the FBO also a quick outcome on the comparison of different materials (based on the technical sheets) provided by one or different suppliers for the realistic conditions of the own packed product. It will allow the FBO to explore rapidly much more choices without additional costs of testing all the materials.

For converters, the software is a valuable addition to the regular testing of different plastic materials on their O_2 permeability. The software can be used to examine the impact of the chosen materials and the material distribution on the permeability of a complete package. Besides, it can also be used as a powerful tool to show the performance of their own material in comparison with other materials in the conditions which are important for the end-users. PredOxyPack® can also be used to determine quickly which factors are affecting the packaging performance the most. In this way, it can help to evaluate which changes to the packaging will result in an acceptable package with all the appropriate characteristics.

For the development of new packages, the majority of physical testing can be completed in a few days; permeability tests, however, can take much longer. This makes the permeation testing one of the largest hurdles in testing new developed packages. PredOxyPack® can help to indicate whether the new packaging concept will perform worse or better than another package regarding the O_2 permeability. With the software tool the user can quickly compare new, innovative packaging materials and make sure that the required O_2 barrier can be achieved. Because of the various options regarding material choices, packaging design, time and temperature combinations, it is possible to explore in a first phase of the development a wide range of packaging options through the software tool. Based on these outcomes, the most promising concept could be analyzed in a second phase with O_2 permeability measurements.

Case study: MAP for fresh fish

For the packaging of fresh fish, PP trays are often used e.g. 500 µm PP and 20 µm PE with an alternative top foil PE/EVOH/PE. Assume that for several reasons, the FBO wants to use a PET/PE tray with the same top foil. The shelf life of the product in the current package is 3 days at 2°C followed by 7 days at 4°C. Based on the simulations of PredOxyPack®, the FBO can easily calculate what will be the difference in O_2 evolution within the headspace for the PP tray and PET tray with the same thickness. From the simulations it is clear that the permeability in the PET tray is much more limited than in the PP tray (Fig. 4 and 5). Even using a thinner PET tray of 300 µm does still give a much better result.

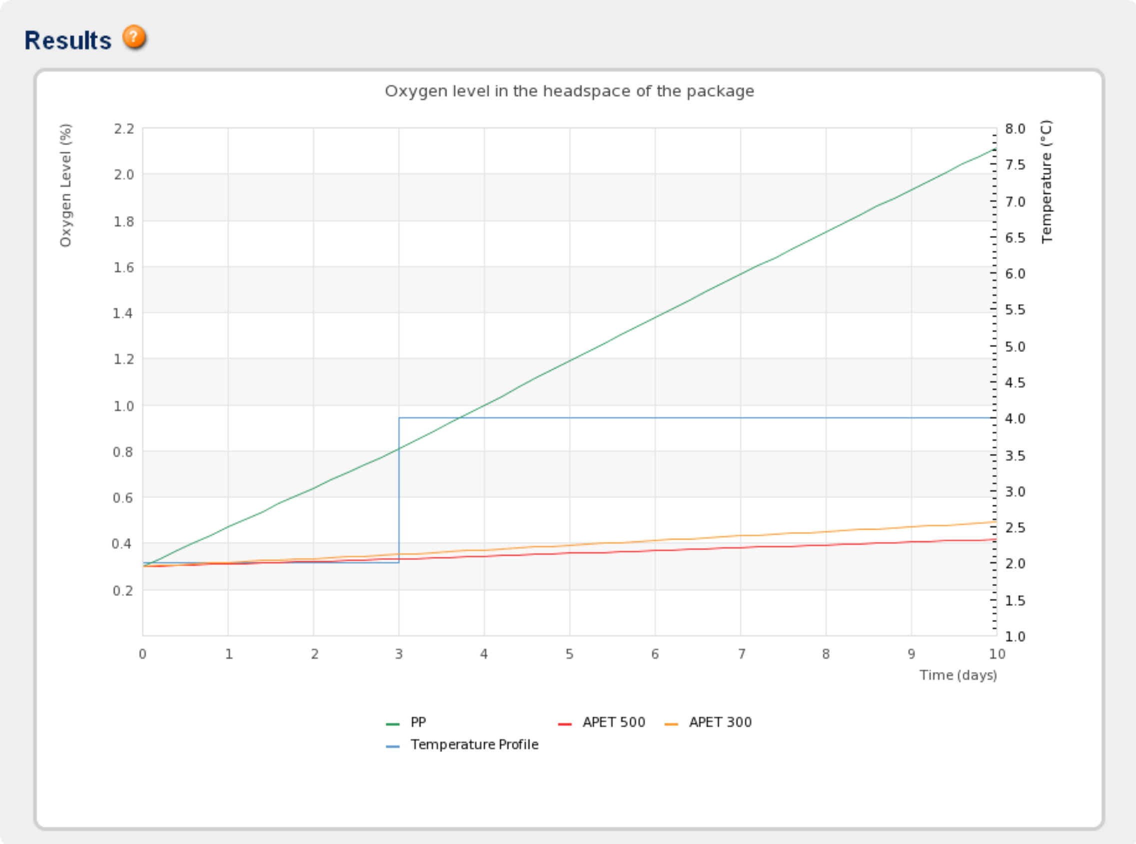

Fig. 4 PredOxyPack® output: % O_2 as a function of time in the headspace of a PP or PET tray with PE/EVOH/PE top film stored for 3 days at 2°C followed by 7 days at 4°C.

rename selected series – clear all series

PP × | APET 500 × | APET 300 ×

Packaging

Geometry	W (width)	H (height)	D (depth)
Tray (Rectangular Cuboid)	20.5 cm	1.5 cm	15.5 cm

Total Volume	Product Volume	Headspace Volume	Initial O_2
477 cc	250 cc	227 cc	0.3 %

Component: Body (425.75 cm²)

Material	OTR	$Thickness_{test}$	$Temperature_{test}$	Thickness
APET	4250 cc/m².day.atm	1 µm	23 °C	300 µm
LDPE	205000 cc/m².day.atm	1 µm	23 °C	20 µm

Component: Top (317.75 cm²)

Material	OTR	$Thickness_{test}$	$Temperature_{test}$	Thickness
LDPE	205000 cc/m².day.atm	1 µm	23 °C	20 µm
EVOH	12.5 cc/m².day.atm	1 µm	23 °C	8 µm
LDPE	205000 cc/m².day.atm	1 µm	23 °C	20 µm

Temperature Profile

Part 1	Part 2
3 days	7 days
2 °C	4 °C

Fig. 5 PredOxyPack® output: Summary of all input variables for the performed simulations

Conclusions

PredOxyPack® is a user-friendly software simulation tool which predicts the headspace oxygen concentration in different packaging configurations and storage conditions. The software enables the user to check or compose a packaging configuration and evaluate the oxygen ingress over time for the realistic storage conditions of the packed product.

Reference

Robertson, G.L. (2006) Food Packaging – Principles and practice (pp. 18-38). New York: Taylor & Francis

Van Bree, I., De Meulenaer, B., Samapundo, S. Vermeulen, A., Ragaert, P., Maes, K.C., De Baets, B. and Devlieghere, F. (2010). *Innovative Food Science & Emerging Technologies 11* (3), 511-519.