

Oxygen Transfer in Co-Extruded Multilayer Active Films for Food Packaging

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Oxygen scavenger applications in flexible food packaging are still limited due to the difficulty to ensure scavenging activity during storage and throughout the product shelf life. To avoid fast inactivation of the scavenger, multilayer active structures can be realized by inserting the active layer between two or more inert layers. In this work, an unsteady-state 1D reaction-diffusion mass transfer model was developed for predicting and optimizing the barrier-to-oxygen performance and the physical configurations of the co-extruded multilayer active films. The film configuration was a three-layers structure composed of polyethylene terephthalate (PET) as external inert layers, and PET with a polymeric oxygen scavenger as the core reactive layer. Scavenging activity of the multilayer film increased with the reactive layer thickness. Oxygen absorption reaction at short times decreased proportionally with the thickness of the external layers. The most appropriate combinations of inert-to-active film thickness were studied and analyzed. © 2017 American Institute of Chemical Engineers AICHE J, 63: 5215–5221, 2017

Keywords: active packaging, modeling, oxygen scavenger, multilayer polymeric film

Introduction

The gas composition of the atmosphere surrounding a packaged food, especially for perishable fruits and vegetables, should be kept at optimal concentrations in order to preserve and minimize deterioration of its quality attributes.^{1–3} Oxygen plays a significant and major role in the deterioration of packaged food products. Its presence provides favorable conditions for the growth of aerobic microorganisms, favors enhanced respiration for fruits and vegetables as well as enzymatic reactions. This could lead to adverse quality deterioration such as loss of ascorbic acid, browning, increased respiration in fruits and vegetables, oxidative rancidity of unsaturated fats, darkening of fresh meat pigments, fostering the growth of mold and aerobic spoilage microorganisms to count only a few. Conversely, inadequate oxygen concentration around the food product could promote the growth of anaerobic pathogens microorganisms, such as *C. botulinum*.⁴

In recent years, active packaging has been preferred over passive packaging due to its versatility and capability to preserve the food product and protect it from external influences that could cause quality losses and deterioration. Polymeric

films with active materials inserted in the package (i.e., scavenger sachets) have been used to extend shelf life and extending its shelf life.⁵ In addition to sachets, oxygen-scavenging compounds can also be incorporated directly into the packaging material itself. These materials include flexible films, rigid plastics (e.g., injection, blow molded polymers⁶) and liners in closures. The development of multilayer films has introduced better barrier performance to achieve the desired packaging requirement according to the unique needs of the food product during storage. Furthermore, the inclusion of scavenger materials in multilayer films in combination with the various processes (e.g., co-extrusion, lamination, coating) have been shown to increase the barrier performance.^{7–11}

The addition of one or more reactive layers in the heterogeneous structure of the packaging provides better barrier properties by reducing permeation rates through the structure, compared to homogeneous barriers. For instance, a multilayer films scavenging activity and the influence of the different concentration of the scavenger on the structure and barrier properties of a polyethylene terephthalate (PET) film loaded with of oxygen scavenger (OS) at 10% showed better oxygen scavenging capacity in comparison with its counterpart PET film.^{12,13}

Carraza et al.⁷ considered the barrier behavior of films composed of a blend of reactive particles and an inert polymer matrix by following the shrinking core model approximation

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of the oxygen permeated in to the packaging material. However, due to the fast reaction process over diffusion, the radius of the reactive core decreased with time and made the shell around it to be thicker. Many other studies, devoted to improve the barrier performance of the multilayer films, pointed out that the barrier properties of multilayer polymeric films could be improved by inclusion of scavenging materials.^{14–16} The configuration of single reactive layer within a multilayer film with different number of inert layers have been also studied,^{8,16} however, there are only limited studies on the analysis of the layers' thickness with respect to the concentration of the scavengers. The specific selection of the polymer that has to be incorporated into the multilayer film depends on the specific requirement of the food product to be packed and its required shelf life. The barrier property of these packaging is highly influenced by the thickness of the polymer and the mass ratio of the scavenging material loaded into the matrix.

In a previous study,¹⁷ three-layers ABA type multilayer polymeric films (A and B represent the inert- and the reactive-layer, respectively) were experimentally produced by a co-extrusion process in order to study the role of the different mass ratio and layer thickness on controlling the scavenging capacity, activity time, and oxygen absorption rate. Carranza et al.¹⁶ described the effect of configuration and the number of layers on the scavenging performance of the films, and pointed out that an ABA type is the preferable configuration for food and pharmaceutical applications. Tung et al.¹⁸ evaluated styrene-butadiene-styrene block copolymer with varying amounts of a cobalt catalyst as an oxygen scavenging component for barrier systems, and recommended a theoretical model to predict the critical thickness of multilayer films from basic principles rather than using the extensive experimental protocols. However, further studies are required in order to optimize the barrier properties considering both OS concentration and layers thicknesses with respect to the packaged food. Indeed, the development of an optimum barrier property and the best configuration of the multilayer polymeric films are the main objective of many recent studies, nevertheless, no validation of the modeling results exists to date.

The overall objectives of this work were:

- developing a user-friendly app for describing the most relevant transport phenomena and predicting the barrier performance of the three-layers polymeric film consisted of two-inert layers and one-reactive layer in the center at different mass ratios with respect to their thickness;
- validation of the aforementioned app, by comparison with experimental data obtained from multilayers samples produced *ad hoc*;
- analyzing the effect of process parameters on the barrier performance and evaluate the design capabilities of the proposed virtual tool.

Material and Methods

Model description and validation procedure

A multilayer polymeric film of a thickness, L and area, A , composed of three-layers (consisting of two-inert layers and one-reactive or scavenging layer) arranged in an alternating pattern was considered in this study. A one-dimensional (1D) transient diffusion in a medium bounded by a container (vial) filled with air, in which all diffusing material enters through the plane faces and negligible amount through edges was assumed. All layers of the film (active- and inert-layers) were

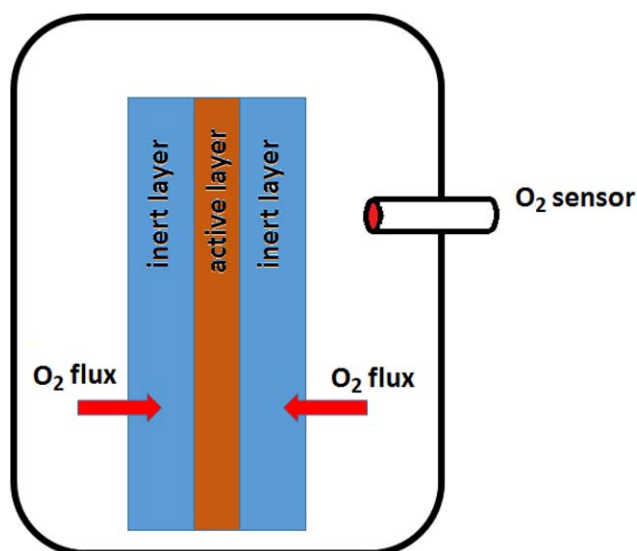


Figure 1. Sketch of the experimental apparatus used to validate the model.

[Color figure can be viewed at wileyonlinelibrary.com]

assumed to be devoid of oxygen concentration at the initial time, while the active film was loaded with oxygen scavenging material at different mass ratios with respect to the thicknesses of the film studied.

In order to validate the model, experimental trials outlined previously¹⁷ were performed. The model was developed and validated in the experimental apparatus depicted in Figure 1, and an ABA symmetrical structure of polymeric films were utilized.

Governing equations

The mathematical description of diffusion in an isotropic medium is based on Fick's first law (Eq. 1), which states that the transfer rate of diffusing substance through a unit area is proportional to the concentration gradient normal to the section:

$$J = -D \frac{\partial C}{\partial x} \quad (1)$$

where, J is the molar flux, D is the diffusion coefficient, C is the concentration of diffusant, and x is the film thickness. Under unsteady state conditions, the three-dimension general equation of the diffusion-reaction across a material can be written as:

$$\frac{\partial C}{\partial t} = D \nabla^2 C + R \quad (2)$$

where t is the process time and R is the rate of reaction considered.

In this study, consumption of oxygen due to scavenging activities has been treated as a pseudo-second order reaction, described in the following expression:

$$R_{oxy} = -k_b^* C_{oxy} \varepsilon \quad (3)$$

where k_b^* is the reaction rate constant, C_{oxy} is the oxygen concentration, as moles per unit of volume, and ε is the number of scavenger moles effectively active, time by time, per unit of

volume, and it is a model variable taking into account the scavenging efficiency, as in the following expression:

$$\varepsilon = \eta C_{sc} \quad (4)$$

where η is the scavenging efficiency defined as moles of active scavenger per moles of scavenger loaded in the active layer, and C_{sc} is the molar concentration of scavenger.

As discussed by Galdi and Incarnato,¹³ high content of scavenger mass in an active film does not correspond always to high scavenging capacity (defined as volume of oxygen, per scavenger mass, that fully reacted up to exhaustion time). In fact, η depends mostly on the scavenger dispersion within the matrix. By following the approach used by Carranza et al.,¹⁶ the mass balance for the oxygen and the scavenging material is expressed by these reported equations:

$$\frac{\partial C_{oxy}}{\partial t} = D_i \frac{\partial^2 C_{oxy}}{\partial x^2} - k_{bi}^* C_{oxy} \varepsilon \quad (5)$$

$$\frac{d\varepsilon}{dt} = -v k_b^* C_{oxy} \varepsilon \quad (6)$$

where v is the stoichiometric coefficient for scavenging reaction and x is the position along the film thickness.

The transient oxygen mass transfer (Eq. 5) accounts for both diffusion and reaction, thus it is described by a partial differential equation; the transient scavenger mass transfer (Eq. 6) is given by an ordinary differential equation. The oxygen mass diffusion coefficient of the i -layer, D_i , is different from layer to layer, according with the constituting material, and so different values were considered since the presence of scavenger and reaction affects the diffusivity of oxygen into the film.¹⁶ The reaction rate constant is null in the inert layers, so that in these portion of the domain the oxygen mass transfer is due only to diffusion. In the scavenger mass balance, no diffusion has been taken into account as well as the products of the reaction were ignored, since there is no diffusion in the layer other than diffusion of the oxygen.

The reaction between oxygen and scavenger material was considered as a pseudo second-order reaction and, as stoichiometry, it was assumed that two molecules of oxygen reacts with one molecule of active scavenger material.⁷ The diffusion of gaseous permeating species into the polymers can also depend on the molecular size, physical state of the diffusant, the morphology of the polymer, and the solubility limit of the solute within the polymer matrix.

The oxygen mass transfer in the experimental vial is described by the following equation:

$$C_{oxy_vial}(t) V_{vial} = C_{oxy_vial}(t=0) V_{vial} - Q(t) A \quad (7)$$

where V_{vial} is the volume of the vial, A is the surface of the multilayer film exposed to mass transfer with the surrounding environment, and $Q(t)$ is the cumulative amount of oxygen permeated per unit area into the film through two external surfaces of PET, defined as follows:

$$Q(t) = \int_0^t J(t)_{x=0} dt \quad (8)$$

Initial and boundary conditions

At initial time condition, no oxygen has been considered in either the inert- and the active-layers. Furthermore, the concentration of the scavenger in the active layer is C_{sc0} . The initial concentration of the oxygen in the vial was calculated

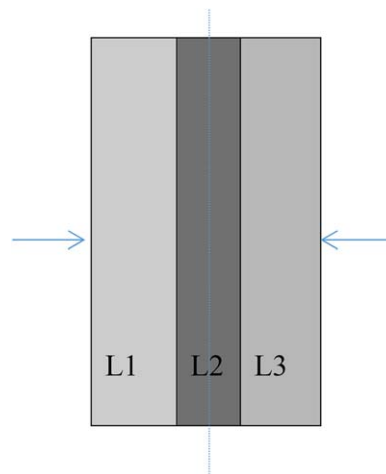


Figure 2. Configuration of multilayer polymeric film used in model, L1, L2, and L3 are the thickness of the three-layers considered in this work.

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according to the ideal gas equation at a temperature of 23°C and total pressure of 1 atm from which the partial pressure of oxygen is 0.21 atm.

The oxygen mass transfer equation requires also boundary conditions. Given the structure of the multilayer film and the configuration of the experimental setup, symmetry of oxygen concentration profile has been set at the middle section of layer 2 (referring to Figure 2), while at external surfaces of the inert films the following condition has been considered:

$$C_{oxy}(0, t) = C_{oxy}(L, t) = s C_{oxy_vial} \quad (9)$$

where $C_{oxy}(0, t)$ and $C_{oxy}(L, t)$ represent the oxygen concentration at system boundary in film side, s is the solubility coefficient of oxygen in the polymer and C_{oxy_vial} is bulk concentration of oxygen in the vial.

Mass balance of oxygen must respect continuity of mass flux at the interfaces between reactive and inert matrix layers, as well as equilibrium partitioning relation, as well explained by Carranza et al.,¹⁶ that constitutes the boundary conditions for the oxygen balance at the interfaces between layers.

Parameter and constants

The parameters and constants used in this work were taken from Di Maio et al.¹⁷ and are listed in Table 1. As discussed by Di Maio et al.,¹⁷ exhausted inert (PET) and active (PET + 10% wt/wt of the active scavenger Amosorb DFC 4020, Colormatrix Europe, Liverpool, UK) exhibit different oxygen solubility values, also as a function of multi-layer film configuration. Conversely, these values remain in a very narrow range (from 6.3×10^{-2} and 7.3×10^{-2} cm³/cm³/bar¹⁷). For this reason, solubility coefficients in the inert and in the active layer were considered to be equal (as in Carranza et al.¹⁶ base calculation).

Numerical solution

The set of differential and integral equations (Eqs. 5–8) was solved using an app built by means of a FEM based commercial software (Comsol 5.0, Comsol AB, Stockholm, Sweden). A multiphysics module for transport of diluted species involving reaction was solved with the initial and boundary

Table 1. Parameters and Constants Used in the Model (Taken from Di Maio et al.,¹⁷, SC = Oxygen Scavenger)

Description	Parameter	Value	Units
Oxygen diffusivity in inert PET matrix	D_m	4.81×10^{-9}	cm^2/s
Oxygen diffusivity in reactive layer	D_r	2.40×10^{-9}	cm^2/s
Volume of head space	V_{hs}	70	mL
Initial concentration of scavenger at $t = 0$	C_{sc0}	1.186×10^{-2}	mol/L
Initial concentration of O_2 at $t = 0$ in the vial	$C_{oxy_vial(t=0)}$	8.561×10^{-3}	mol/L
Solubility coefficient	S	7.16×10^{-2}	$\text{cm}^3/\text{cm}^3/\text{bar}$
Area	A	25	cm^2
Reaction rate constant	k_b	1×10^4	$\text{cm}^3/(\text{mol s})$
Stoichiometric factor	N	2	mol of O_2 /mol of SC

conditions listed above. General steps for developing the app in Comsol 5.0 require the definition of the mathematical system, the definition of the parameters and the variables, the system geometry, defining the different subdomains, the assignment of initial and boundary conditions, choosing the proper mesh and post processing of the results.

In order to analyze the influence of the film configurations and process parameters on the barrier performance of the films, parametric study was utilized for different thicknesses of the layers and parameters. The effect of different film thicknesses of inert and reactive layers, keeping the overall film thickness as constant, with respect to relative mass ratios of the loaded scavenger material was evaluated and compared with the experimental data. In addition, the effect of diffusivity and rate of reaction was also analyzed by varying the coefficients using the values reported previously¹⁷ as a base value.

Experimental

The ABA type symmetrical structure polymeric films were considered for this study. Of the three-layers, the middle layer was made up of PET polymer loaded with 10% of active OS material, while the external layers were pure PET. The active OS selected was Amosorb DFC 4020 (AMS, supplied by Colormatrix Europe, Liverpool, UK), a co-polyester based polymer designed for production of rigid PET containers. The multilayer films at different mass ratio of scavenger concentration were produced in the laboratory following the process and operating conditions described previously.¹⁷ Monolayer films made of PET and active PET (10% wt/wt of AMS) were also considered in the study for comparison. The relative mass ratio of the co-extruded multilayer and monolayer films, with respect to their thickness (in μm) are listed in Table 2.

Results and Discussion

Oxygen depletion in the vial

Before discussing the simulation results, it is useful to know what are the characteristics of experimental oxygen concentration depletion in the vial, equipped with three-different

configurations of multilayer active packages denoted: ML1, ML2, and ML3. As show in Figure 3, after a quick oxygen depletion in the first hours for all the three-considered configurations, one can notice that after a certain period of time (different case by case, during which the oxygen in the vial continues to be consumed by the OS loaded in the multi-layers film), oxygen concentration in the vial reaches a final constant value. This time, denoted “exhausting time,” can be determined from the graph depicted in Figure 3, when the slope of the experimental curve is approaching zero. For instance, for ML1 configuration, the exhausting time is 196 h after which the oxygen concentration in the vial remains at 6.56 (mol/ m^3). For ML2 and ML3 configurations, the oxygen concentration in the vial reaches a plateau of 5.55 (mol/ m^3) and 4.55 (mol/ m^3) after 347 and 432 h, respectively. Obviously, in an ABA scheme, given the same mass of scavenger loaded in the active layer, the thicker the inert layer is the longer will be the time needed to achieve a stationary value of oxygen in the vial. This is due to the fact that before encountering the OS, the oxygen has to diffuse into the inert layers. Furthermore, going from ML1 to ML3 configurations, the mass of OS loaded in the active layer increases: this allows consuming larger amount of oxygen, thus more oxygen molecules were depleted from the vial volume toward the active layer with the OS properties.

Exhausting time (of the three-different configurations experimentally studied), the corresponding final percentage of oxygen are key-parameters that have been used also to discuss the validation of the proposed model (Table 3).

Model validation

In order to validate the proposed model, two separate comparisons were carried out: a comparison between the oxygen concentration and evolution time predicted by the model and the corresponding data that were obtained experimentally.

Figure 3 depicts the model prediction for ABA configurations of ML1 (continuous line), ML2 (dotted line), and ML3 (dashed line). The predicted data was then compared with the experimental time evolution of oxygen concentration in the vial, referred to the same ABA configurations. The trends of time evolution of oxygen concentration in the vial provided by the model numerical solution are in close agreement with the experimental data, except for some initial discrepancy observed probably due to the fast oxygen depletion in the first 10–20 h of the process. For configuration ML1, the agreement between the numerical simulation and the experimental data is excellent, both in terms of the time evolution of oxygen concentration in the vial and the exhausting time of 195 h, which is in very close agreement with the 196 h estimated from the experimental data, and, the final value of oxygen concentration in the vial. The oxygen concentrations calculated by the

Table 2. Relative Mass Ratio and Thickness of the PET Layers (Di Maio et al.,¹⁷)

Film description	Relative mass ratios	Thickness of the layers L1/L2/L3 (μm)
	External layer/ core layer (%/%)	
SL-PET	100/0	17.5/0/17.5
ML1	70/30	13.0/9.0/13.0
ML2	60/40	10.75/13.50/10.75
ML3	50/50	9.0/17.0/9.0

SL-PET, Single Layer of PET.

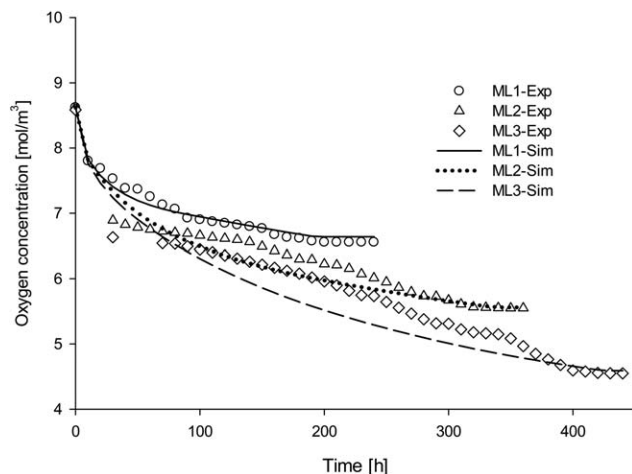


Figure 3. Comparison between simulated and experimental time evolution of oxygen concentration in a vial equipped with ML1, ML2, and ML3 configuration.

model were 6.64, 5.59, and 4.59 (mol/m^3) (vs. 6.56, 5.55 and 4.55 mol/m^3 estimated experimentally) were obtained for the ML1, ML2, and ML3 configuration, respectively.

In terms of comparison of exhausting time and final oxygen concentration in the vial, Figure 3 and Table 2 show a good agreement between the simulated and experimental values, in all tested cases. The model however, predicts in comparison with the experimental data, a slightly shorter exhausting time (less than 5% discrepancy) for all the configurations considered. Conversely, as expected, slightly higher values of oxygen percentage in the vial were derived by the simulation in comparison with the experimental estimation (less than 3% discrepancy). Based on these data, it is possible to conclude that the proposed model could be used to predict quite accurately the exhausting time and the maximum amount of oxygen that the active multilayer film can treat, configuration by configuration. Carranza et al.¹⁶ have proposed analytic predictions for the so-called time lag, which is close to the exhaustion time previously discussed. It is quite interesting to note that the analytical prediction proposed by Carranza et al.¹⁶ (obtaining their analytical correlation using a completely different system much wider thickness, and different boundary conditions) provided time lag values higher than the exhausting times experimentally and numerically derived, nevertheless, still quite comparable (i.e., time lag values of 250, 430, and 585 h for configurations ML1, ML2, and ML3, respectively). Once the model has been validated, it can be also utilized to analyze the time evolution of oxygen profiles inside an active multilayer configuration.

Table 3. Comparison of Exhausting Time and Final Oxygen Concentration, for the Three ABA Configurations Considered (exp, Experimental; sim, Simulated)

Configuration	ML1		ML2		ML3	
	exp	sim	exp	sim	exp	sim
Exhausting time (h)	196	195	347	331	432	422
Final oxygen concentration (mol/m^3)	6.56	6.64	5.55	5.59	4.55	4.59

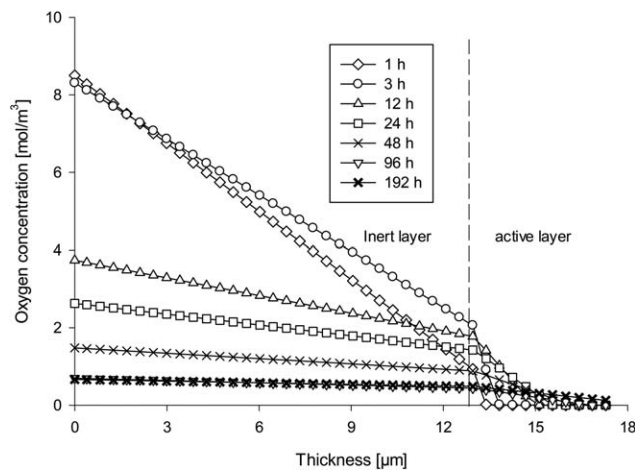


Figure 4. Simulated time evolution of oxygen concentration profiles inside the multilayer film, in an ABA ML1 PET/active/PET configuration.

Transient of oxygen concentration profile in the film matrix in the ML1 configuration

Figure 4 depicts the first hours during which the active multilayer is exposed to a low oxygen concentration atmosphere (3%) is at the interface with the scavenging layer since every molecule of oxygen reaching the OS is consumed. The oxygen moves from the vial volume through the active multilayer film toward its middle layer (where the scavenger is). While the oxygen enters the multilayer film, the gas volume of the vial occupied by the oxygen decreases and, consequently, also the concentration of oxygen at the boundary between the multilayer film and the vial environment. Already after 12 h, the concentration of oxygen on the external surface of the multilayer film is less than the half of its initial value. Between 12 and 48 h, the OS layer has to consume the oxygen that diffused, and after 192 h there is still some active scavenging area inside the film.

Role of initial concentration of scavenger

The derived model (after its validation), was used to study the effects of a number of design parameters on the performances of the active multilayer film.

The scavenging activity in the active layer is mainly dependent on the amount of OS concentration loaded in the matrix (i.e., the number of active sites found in the matrix of the film). This characteristic was determined by inverse modeling technique using experimentally measured values reported previously (Galdi and Incarnato,¹³ and Di Maio et al.¹⁷). It is obvious that the wider the thickness of the inert layer the higher is the number of active sites.

Under the hypothesis that the OS can be uniformly loaded into an active layer, as in the ML1 configuration, one has a certain estimation of the initial amount of effective scavenger material per unit of volume (C_{sc0}), the model has been used to predict the film performance when the initial amount of effective scavenger material per unit of volume was doubled (i.e., two C_{sc0}) or quadrupled (i.e., four C_{sc0}), as depicted in Figure 5. It should be noted that, the OS concentration loaded in the matrix also determines the barrier performance. It is possible to appreciate that, while with an initial amount of effective scavenger material per unit of volume C_{sc0} , the final

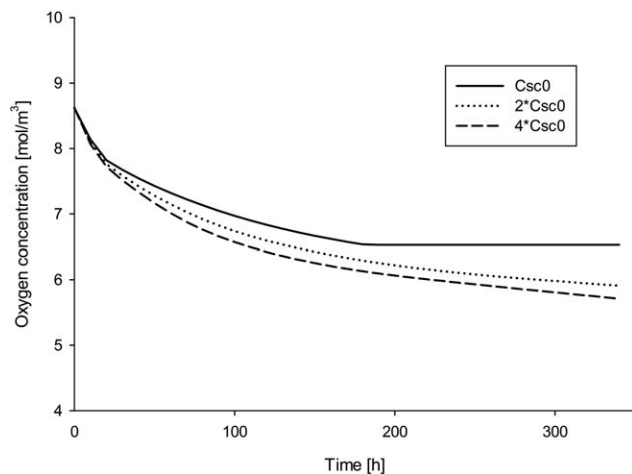


Figure 5. Comparison of simulated time evolution of oxygen concentration in the vial when initial concentration of OS loaded in the active layer is Csc0 (continuous line), 2 Csc0 (dotted line), and 4 Csc0 (dashed line), in a ABA ML1 PET/active/PET configuration.

value of oxygen concentration in the vial is $6.64 \text{ (mol/m}^3\text{)}$ obtained after an exhausting time of about 195 h. When this amount of effective OS material is doubled (two Csc0), the depletion of oxygen is still ongoing after 350 h. The slopes (oxygen concentration/h) varied from -4.4×10^{-3} to -5.7×10^{-3} for two Csc0 and four Csc0, respectively. The higher the OS concentration loaded in the matrix, the longer is the time to reach oxygen concentration plateau.

Of course, there are physical and processing limits (because of constraints imposed by the film extrusion itself) above which no additional OS can be loaded into the active film or when—even adding a larger amount of scavenger—there is no effect on the OS capacity of the active film due to scavenging agglomeration or its poor dispersion in the matrix (as already demonstrated by Galdi and Incarnato¹³).

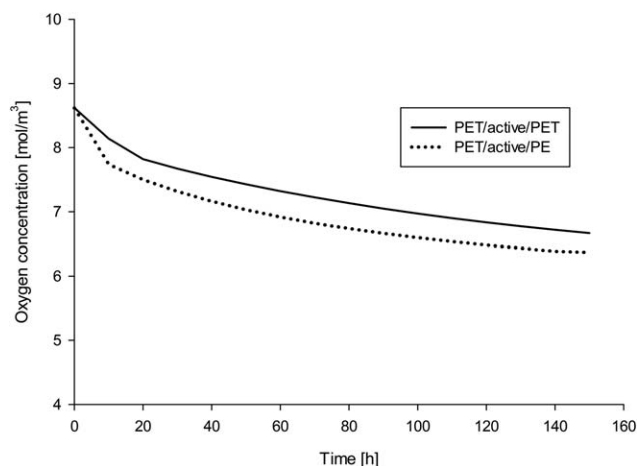


Figure 6. Comparison between simulated time evolution of oxygen concentration in the vial with a ABA ML1 PET/active/PET or a ABC ML1 PET/active/PE configuration.

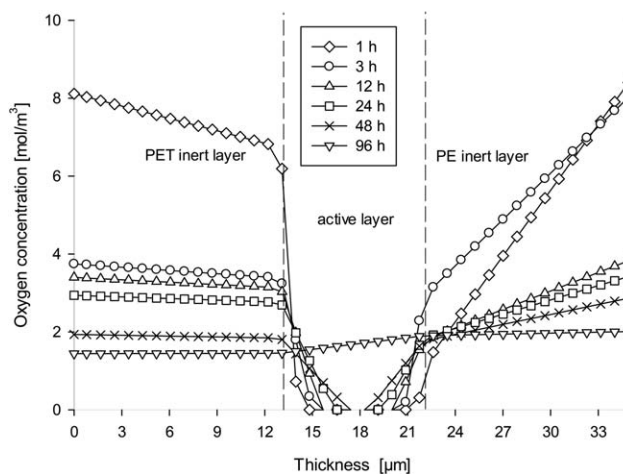


Figure 7. Time evolution of oxygen concentration profiles inside the multilayer film of ABC ML1 configuration of PET/active/PE.

ABA scheme (PET/active layer/PET) vs. ABC configuration (PET/active layer/PE)

The derived model can be further utilized to predict the behavior of a film in the case of an ABC scheme, as in the case of active layer sandwiched between an inert layer of PET and an inert layer of PE, holding the same thicknesses as in configuration ML1 and the same active layer characteristics.

ABC scheme, depletion of oxygen percentage in the vial

The overall effect of this ABC combination can be demonstrated in Figure 6, where the depletion of oxygen concentration in the vial is plotted versus time. The data related to the ABA scheme (PET/active layer/PET) are reported as a continuous line, while ABC scheme (PET/active layer/PE) data are represented by the dotted line. The ABC scheme produces a quicker depletion of oxygen but only up to 146 h. From this time, the OS is exhausted and any other further exposition of the film to oxygen sources will result in an increase of the oxygen content in the film itself. The ABA scheme is more effective, since its exhausting time was 195 h, thus almost 34% higher than the counterpart predicted for the ABC scheme.

Effect of layer composition on the transient of oxygen concentration profile in the film matrix in the ML1 configuration

Oxygen depletion profiles with time is depicted in Figure 7, where the PE layer and PET layer is listed on the right and left side, respectively. PE oxygen profiles differ from the counterparts in the PET. This is first due to the different diffusivity of the oxygen in the polymers (4.81×10^{-13} and $5 \times 10^{-12} \text{ m}^2/\text{s}$, for PET and PE, respectively¹⁷). The higher decreases the resistance to mass transfer and consequently the oxygen that reaches the boundary with the active layer exhibits higher concentration, resulting in a faster depletion. The different diffusivity values produce an asymmetrical plot, from which it is evident that, after 192 h, the scavenger activity has disappeared, as the profiles taken at this time (line with circles indicators) is determined by diffusion in a composed slab.

Conclusions

The mass diffusion/mass reaction computational model presented in this study adequately simulated the performances of active multilayer films with OS capacity, both in terms of oxygen concentration depletion with time, and the prediction of the concentration at exhausting time. After validation, the model was utilized to predict the behavior of active multilayer films under different symmetrical ABA configurations, which highlights the importance of the inert to active thickness ratio, and the initial OS loading in the film matrix on the performance of the active film itself. Optimal exhausting times could be obtained by determining the most appropriate combination of inert-to-active film thickness as well as by choosing the most appropriate mass of scavenger to be loaded in the inner active layer. The model could also be utilized for analyzing the performances of more general ABC film configurations, when one of the inert layers is replaced by another polymer (e.g., PE replacing PET).

Acknowledgment

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