Research, Society and Development, v. 14, n. 7, e10414749151, 2025
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Numerical modeling of an active package – a theoretic study

Modelagem numérica de uma embalagem ativa – um estudo teórico

Modelado numérico de un paquete activo – un estudio teórico

Received: 06/24/2025 | Revised: 07/28/2025 | Accepted: 07/29/2025 | Published: 07/31/2025

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Abstract
This article presents an analytical-numerical study of active food packaging is presented. Such packages have in their compositions materials through which oxygen may flow in both directions (from inside to external environment and vice versa), or just one (vaccum inside) and models describing this problem are usually formulated as coupled nonlinear partial differential equations. The main contribution of this paper is to show that a solution can be obtained from a well-known model using free software, following a combined analytical and numerical approach. The results obtained suggested that such an approach is valid and may lead to further developments in more accurate modeling. Our focus in this research is not to analyze what happens to the food contained in these packages, their practical uses, or their possible ecological and financial impacts on the food industry. We are focused on how to simulate these packages and collaborate with the research process on them.
Keywords: Absorber layer; Oxygen barrier; Numerical model; FORTRAN 77.

Resumo
Neste artigo, é apresentado um estudo analítico-numérico de embalagens ativas de alimentos. Tais embalagens possuem em sua composição materiais pelos quais o oxigênio pode fluir em ambas as direções (de dentro para o ambiente externo e vice-versa), ou apenas em uma (vácuo no interior), e os modelos que descrevem esse problema são geralmente formulados como equações diferenciais parciais não lineares acopladas. A principal contribuição deste artigo é mostrar que uma solução pode ser obtida a partir de um modelo bem conhecido por meio de software livre, após uma abordagem analítica/numérica combinada. Os resultados obtidos sugerem que tal abordagem é válida e pode levar a futuros desenvolvimentos em modelagem mais precisa. Nosso foco principal neste trabalho não é analisar o que acontece com os alimentos contidos nessas embalagens, seus usos práticos ou seus possíveis impactos ecológicos e financeiros na indústria alimentícia. Estamos focados em como simular essas embalagens e colaborar com o processo de pesquisa sobre elas.
Palavras-chave: Camada absorvedora; Barreira ao oxigênio; Modelo numérico; FORTRAN 77.

Resumen
En este artículo se presenta un estudio analítico-numérico de envases activos para alimentos. Dichos envases contienen en su composición materiales a través de los cuales el oxígeno puede fluir en ambas direcciones (del interior al exterior y viceversa), o solo en una (vacío en el interior), y los modelos que describen este problema suelen formularse como ecuaciones diferenciales parciales no lineales acopladas. La principal contribución de este artículo es mostrar que se puede obtener una solución a partir de un modelo conocido mediante software libre, tras realizar un enfoque analítico/numérico combinado. Los resultados obtenidos sugieren que dicho enfoque es válido y puede conducir a futuros desarrollos en modelos más precisos. Nuestro principal objetivo en este trabajo no es analizar qué sucede con los alimentos contenidos en estos envases, sus usos prácticos o sus posibles impactos ecológicos y financieros en la industria alimentaria. Nos centramos en cómo simular estos envases y colaborar con el proceso de investigación sobre ellos.
Palabra clave: Capa absorbente; Barrera de oxígeno; Modelo numérico; FORTRAN 77.

1. Introduction

The packaging of a food product go far beyond its simple conservation function and general information display (nutritional facts, expiration date, storage conditions and handling, among others): it also bears (although this is not visible) physical and chemical properties which help increasing the time this product will be available to the customer. Trying to reach this goal, industry developed new materials and technologies in order to lower interaction levels between food and package itself. Such efforts lead to the so-called *active packaging* which contains materials capable of absorb harmful elements to food, like oxygen. Other packaging methods use substances that reduce odors or have antioxidant/antimicrobial effects (Viana, 2022).

Active packaging systems (Gaikwad, 2018) consist of multiple layers (generally three), with outer and inner layers made of inert materials and middle layer made of a reactive material (Realini, 2014). Polymers like LDPE (low density polyethylene), LLDPE (linear low density polyethylene), HDPE (high density polyethylene), PP (polypropylene), PET (poly[ethylene terephthalate]), PEN (poly[ethylene naphthalate]), PVC-U ([unplasticized] poly[vinyl chloride]), PVdC (poly[vinylidene chloride]), PS (polystyrene), EVOH (ethylene vinyl alcohol copolymers) and PA6 (polyamide 6 UV, ultraviolet) are typical choices (VIANA, 2022) because they all have well-defined physicochemical properties. For instance, PET is an inert material and EVOH is an excellent oxygen flow blocker (VIANA, 2022). A comprehensive review of this type of packaging is found in Kadirvel (2025).

Modern software enables cost reduction by allowing many tests to be computer-simulated instead effectively carried out in a laboratory, thus optimizing the product life cycle and its manufacturing processes. Oxygen flow through package's layers is a phenomenon that can be fully computer-implemented and plays a fundamental role in today's packaging technology.

The literature on this topic is quite extensive, but its main characteristic is the use of commercial (paid) software in solution building. Bedani *et al.* (2015) compared experimental and simulated (COMSOL®) results of a thin film (PET /absorber/ PET). Ferrari *et al.* (2009) used MATLAB® in modeling a multilayer thin film with an oxygen absorbing layer. Their goal was to increase the permeability barrier for this gas. Finally, Carranza *et al.* (2012), using both analytical and numerical approaches in MATLAB®, developed a robust model to study a n-layered system, alternating active and inert layers.

The present framework shows a way to solve numerically a nonlinear multilayer problem described in next section, using traditional numerical methods and free computer tools. Such an approach allows extensive control of the computations and thus greater reliability of the results. The main contribution of this paper is to show that a solution can be obtained from a well-known model using free software, following a combined analytical and numerical approach.

2. Methodology

Following the model proposed by Di Maio (2017), the initial assumption is that the package is composed of three different layers (namely **1**, **2** and **3**) and oxygen flow is one-dimensional (along the horizontal direction in a Cartesian coordinate system). Outer layer 1 and inner layer 3 are made of the same material and central layer 2 absorbs oxygen. The mathematical model is as follows:

$$\frac{\partial C_1(x,t)}{\partial t} = D_1 \frac{\partial^2 C_1(x,t)}{\partial x^2}, 0 < x \leq a, t > 0 \quad [1]$$

$$\frac{\partial C_2(x,t)}{\partial t} = D_2 \frac{\partial^2 C_1(x,t)}{\partial x^2} - kC_2(x,t)\epsilon, a < x \leq b, t > 0 \quad [2]$$

$$\frac{\partial C_3(x,t)}{\partial t} = D_3 \frac{\partial^2 C_3(x,t)}{\partial x^2}, b < x \leq d, t > 0 \quad [3]$$

and

$$\frac{\partial \epsilon(x,t)}{\partial x} = -\nu k C_2(x,t)\epsilon \quad [4]$$

In each layer i ($i = 1,2,3$), the functions $C_i(x,t)$ and D_i represent, respectively, the oxygen concentration and diffusion coefficient at position x and time t. Constants k and ν are, by their turn, the reaction and stoichiometric coefficient of oxygen. Finally, ϵ is the oxygen concentration in the reactive layer, whose rate decreases with time according to eq. [4].

The boundary and initial conditions are:

$$C_1(0,t) = C_3(d,t) = sC_{ext} \quad [5]$$

$$C_1(a,t) = C_2(a,t) \quad [6]$$

$$C_2(b,t) = C_3(b,t) \quad [7]$$

$$D_1 \frac{\partial C_1(a,t)}{\partial x} = D_2 \frac{\partial C_2(a,t)}{\partial x} \quad [8]$$

$$D_2 \frac{\partial C_2(b,t)}{\partial x} = D_3 \frac{\partial C_3(b,t)}{\partial x} \quad [9]$$

$$C_1(x,0) = C_2(x,0) = C_3(x,0) = 0 \quad [10]$$

In [5], parameter s is the oxygen solubility coefficient in the layered material and C_{ext} is the oxygen concentration in the environment outside the package. Equations [6] to [9] stablish the continuity of O_2 flow through layers interface. Finally, equation [10] is the initial condition (*i.e.*, at $t = 0$ there is no oxygen inside the package).

A single glance at equations [1] to [4] makes clear their nonlinear characteristics and the need of applying the suitable mathematical approach to solve them. Hence, equations [1] to [4] were discretized as:

$$T_i^{j+1} = \frac{D_r \Delta t}{\Delta x}\left(T_{i+1}^j - 2T_i^j + T_{i-1}^j\right) + T_i^j\left(1 - k\nu H_r \Delta t Y_i^j\right), r = 1,2,3 \quad [11]$$

$$Y_i^{j+1} = Y_i^j\left(1 - k\nu \Delta t T_i^j\right) \quad [12]$$

T and Y are respectively discretizations of functions $C(x,t)$ (equations [1]–[3]) and $\epsilon(x,t)$ (equation [4]). Note that $H_1 = H_3 = 0$ and $H_2 = 1$. The subscripts j and i relate to time and space respectively.

Including perfect contact conditions (equations [8] and [9]) requires an expansion of functions $C_i(x,t)$ around the points $x = a$ (from right) and $x = b$ (from left), leading to:

$$C_i(x + \Delta x, t) = C_i(x,t) + C_i'\Delta x + \frac{C_i''(\Delta x)^2}{2} \quad [13]$$

$$C_i(x - \Delta x, t) = C_i(x,t) - C_i'\Delta x + \frac{C_i''(\Delta x)^2}{2} \quad [14]$$

Therefore, equation [8] turns into:

$$D_1 \frac{\partial C_1}{\partial x} = D_1\left[\frac{C_1(x,t) - C_1(x - \Delta x, t)}{\Delta x} + \frac{\Delta x}{2D_1}\left(\frac{C_1(x,t + \Delta t) - C_1(x,t)}{\Delta t}\right)\right] \quad [15]$$

$$D_2 \frac{\partial C_2}{\partial x} = D_2\left[\frac{C_2(x + \Delta x, t) - C_2(x,t)}{\Delta x} + \frac{\Delta x}{2D_2}\left(\frac{C_2(x,t + \Delta t) - C_2(x,t)}{\Delta t}\right)\right] \quad [16]$$

In the two equations above, the second term of the derivative in space variable x was replaced by the derivative in time variable t (ASCHER, 1960). For equation [9], one obtains:

$$D_2 \frac{\partial C_2}{\partial x} = D_2\left[\frac{C_2(x,t) - C_2(x - \Delta x, t)}{\Delta x} + \frac{\Delta x}{2D_2}\left(\frac{C_2(x,t + \Delta t) - C_2(x,t)}{\Delta t}\right)\right] \quad [17]$$

$$D_3 \frac{\partial C_3}{\partial x} = D_3 \left[\frac{C_3(x+\Delta x,t) - C_3(x,t)}{\Delta x} + \frac{\Delta x}{2D_3} \left(\frac{C_3(x,t+\Delta t) - C_3(x,t)}{\Delta t} \right) \right] \quad [18]$$

Equating, in pairs, equations [15]/[16] and [17]/[18], the discrete Fourier conditions (perfect contact) become:

$$T_i^{j+1} = T_i^j + \frac{D_m \Delta t}{(\Delta x)^2} \left[T_{i+1}^j - T_i^j \right] + \frac{D_{m-1} \Delta t}{(\Delta x)^2} \left[T_{i-1}^j - T_i^j \right], m = 2,3 \quad [19]$$

In [19], the factor $D_m\,\Delta t/(\Delta x)^2$ is known as Courant number and the stability of numerical solution is guaranteed when $D_m\,\Delta t/(\Delta x)^2 < 0.5$ (ISERLES, 2018). But, in this problem, we will have three different Courant values: which one should be used? Ascher (1960) outlines a method for dealing with this problem, consisting of:

i) choose the value of the spatial discretization Δx;

ii) calculate $\Delta t = \min_{r=1,2,3} \{(\Delta x)^2/[2D_r]\}$;

iii) use equation [11] to get O_2 concentration in material 1;

iv) use equation [19] to get O_2 concentration at interface 1;

v) use equation [11] once again to get O_2 concentration in material 2;

vi) use equation [19] one more time to get O_2 concentration at interface 2;

vii) update Y (equation [12]) and

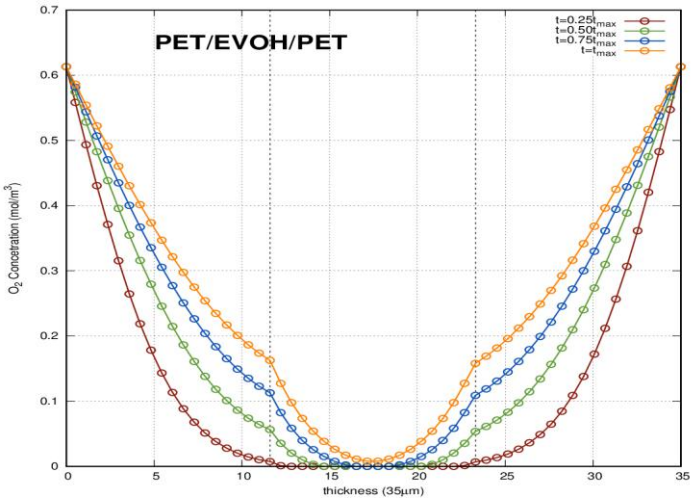
viii) use equation [11] for the last time to calculate O_2 concentration in material 3.

Following this algorithm, we developed a program using the Fortran77 programming language for the Linux operating system. The choice of this language is based on its recognized numerical power, that is, the codes developed in it. In fact, this programming language has already been tested by us in several other studies and it has proven to be very effective (Silva, 2024, Viana 2023, Wanzeller, 2023).

3. Results and Discussion

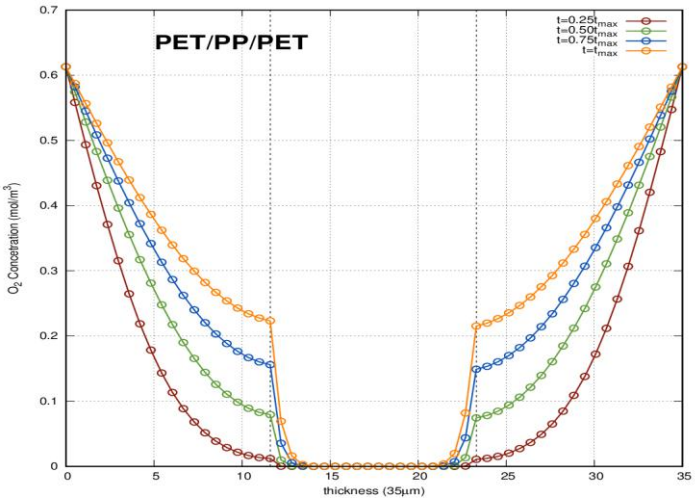
The object of study was a 35mm thick package, divided into three equal segments. We use the following material combinations: PET/EVOH/PET, PET/PP/PET, PET/EVOH/PE and PS/VVC/PE. The oxygen diffusivity (D) in the studied materials are Di Maio (2017), Keller (2017): (cm^3/s): 2.7 x 10^{-9} (PET); 7.2 x 10^{-10} (EVOH); 3.76 x 10^{-7} (PP); 1.01x10^{-6} (PE); 3.1 x 10^{-7} (PS) and 1.01 x 10^{-7} (VCC). The initial concentration O_2 [C_{ext}, (mol/L)] and the Solubility coefficient [s, (cm^3/cm^3/bar)] are, respectively, 8.56 x 10^{-2} and 7.16 x 10^{-2}. First, we deal with a package with the same amount of oxygen in both regions (non-vacuum). Then we consider the absence of oxygen inside the package (x = 35mm), i.e., a vacuum-packed product.

Figure 1 - Oxygen concentration profiles within three studied packages. These packages have an ABA symmetry. The combination of materials used is PET/EVOH/PET.



Source: Authors.

Figure 2 - Oxygen concentration profiles within three studied packages. These packages have an ABA symmetry. The combination of materials used is PET/PP/PET.

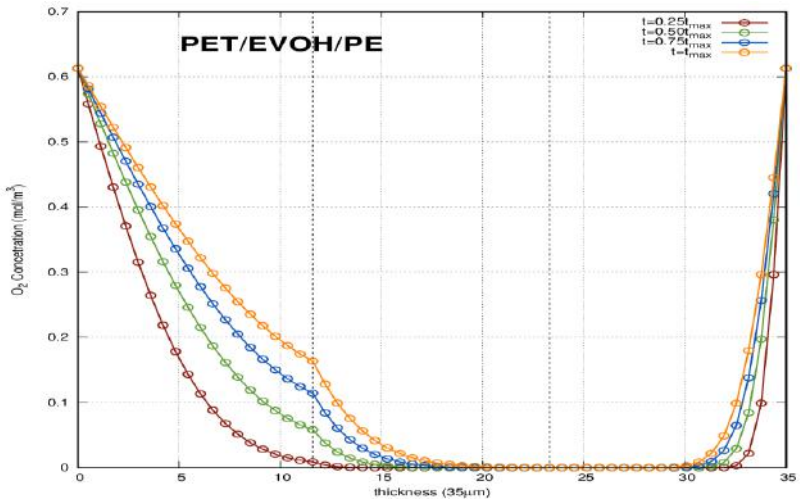


Source: Authors.

3.1 Non-vacuum packaging

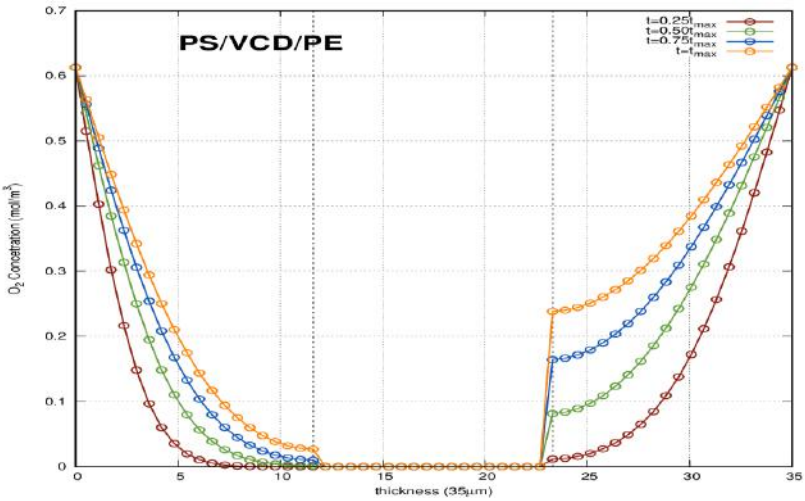
In Figures 1 and 2 we have the ABA arrangements and at Figures 3 and 4 the ABC arrangements. Each combination of materials used is indicated at the top of the graphics. The total simulation time (t_{max}) was 9900 seconds.

Figure 3 - Oxygen concentration profiles within three studied packages. These packages have an ABC symmetry PET/EVOH/PE.



Source: Authors.

Figure 4 - Oxygen concentration profiles within three studied packages. These packages have an ABC symmetry PET/VCD/PE.



Source: Authors.

The ABA profiles present symmetry, from the point of view of the materials involved. Thus, the oxygen concentration profiles within these combinations were expected to be symmetrical. Figures 1 and 2 shows just that. On the other hand, the asymmetry of the materials in the ABC profiles results in an asymmetry in the oxygen concentration inside of the material, and this is found in Figures 3 and 4.

3.2 Vacuum packaging

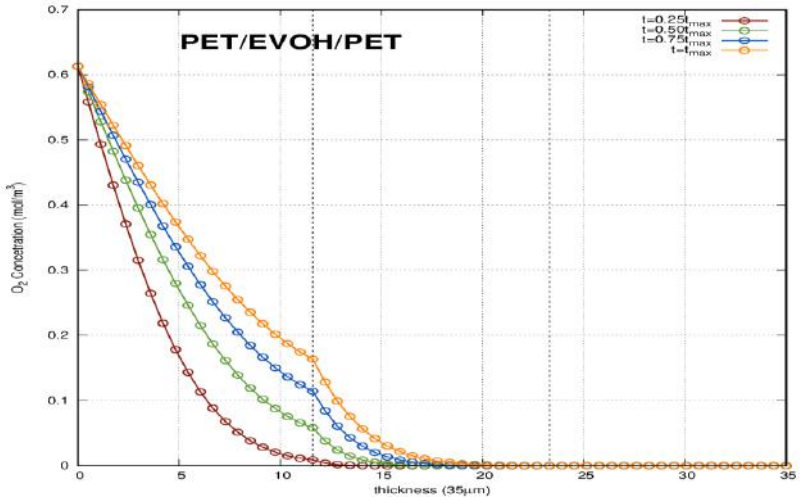
A vacuum package consists of a system in which there is no oxygen inside. For this, the boundary condition must be

$$C_1(0,t) = sC_{ext} \quad [20]$$

$$C_3(d,t) = 0 \quad [21]$$

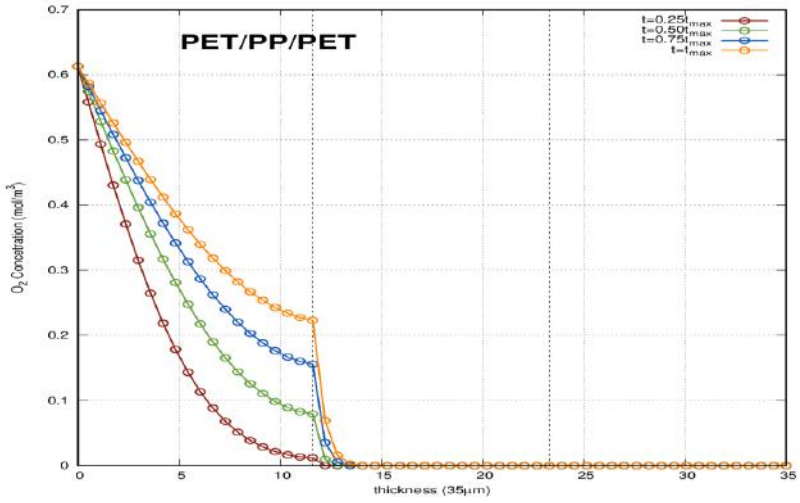
We used the same ABA and ABC settings as before and kept the same thickness and initial condition. In Figures 5 and 6 we have the ABA arrangements and at Figures 7 and 8 the ABC arrangements. Each combination of materials used is indicated at the top of the graphics. The total simulation was held at 9900 seconds. Our results make clear the robustness of the algorithm. It is capable of simulating different packaging configurations in different scenarios (initial conditions). We can also notice that, in both types of material profiles and initial conditions, the oxygen barrier (central layer) was effective, decreasing, and even zeroing, the oxygen concentration. In fact, for the symmetrical arrangement PET/PP/PET and the two non-symmetrical arrangements studied, no oxygen was found in the center of the package. The vertical dashed lines in both figures represent the interface points between the materials. With the aid of these ones, we notice the change in the behavior of the oxygen concentration when the media are changed. This scenario confirms our model.

Figure 5 - Oxygen concentration profiles within three studied packages with vaccum internal and ABA symmetry. The combination of materials used is PET/EVOH/PET.



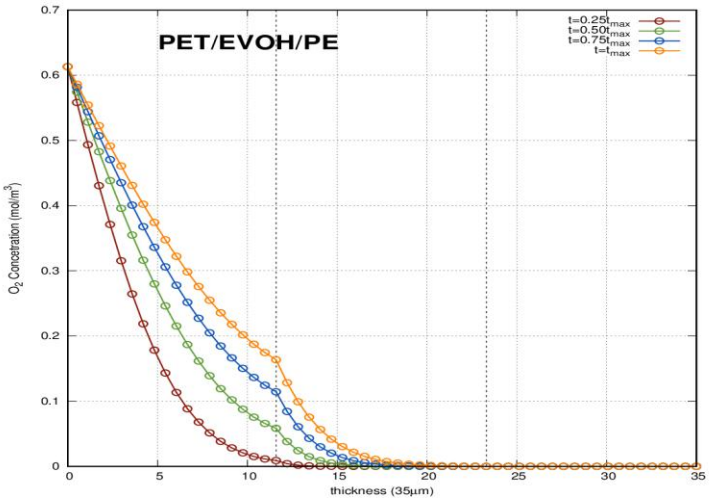
Source: Authors.

Figure 6 - Oxygen concentration profiles within three studied packages with vaccum internal and ABA symmetry. The combination of materials used is PET/EVOH/PET.



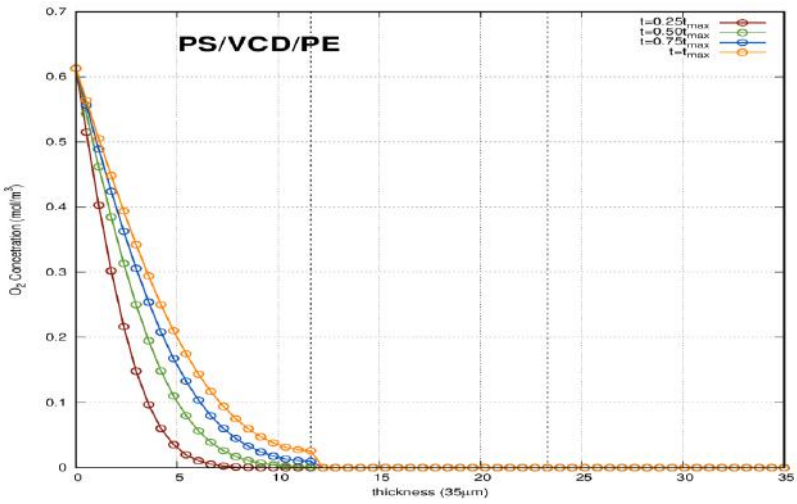
Source: Authors.

Figure 7 - Oxygen concentration profiles within three studied packages with vacum internal and ABC symmetry PET/EVOH/PE.



Source: Authors.

Figure 8 - Oxygen concentration profiles within three studied packages with vacum internal and ABC symmetry PS/ VCD/PE.



Source: Authors.

We used free software Grace (Grace) to plot the graphs. This is a great software option for plotting data on a two-dimensional plane. Emphasizing that one of the main focuses of this article is to show that it is possible to study an active packaging using only free software, well-established numerical methods and a classical programming language.

4. Conclusion

We proposed to develop a numerical code that would allow the study of an active package using free computational tools and traditional numerical methods. Our results show that the objective was satisfactorily achieved. The code may be used

in many ABA and ABC packaging configurations in the future, we should emphasize that this modeling can easily be used in the study of smart packaging, for example, following the mathematical model described by Villas C (2020). In fact, we are currently implementing this study with new pathogenic controls (Bautista-Baños, 2025).

This study, and its results, make it clear that a high investment (software and hardware) is not necessary to model active packaging. We only use free software on a PC configured with the Ubuntu 20.04 operating system, Intel i7 processor and 16GB of RAM memory. We also use free software to plot the results (Glace). We did not use subroutines or closed computational packages, such as Matlab (MATLAB), COMSOL (COMSOL), among others. This gave us total control of the code, and a broad knowledge of how the simulation was done. The use of closed software causes, in our opinion, a lack of control over the simulation. Note that Vilas (2020) used Matlab in his modeling (ZENODO).

Something that requires attention is the discontinuity of the solution function $C_i(x,t)$ at the interface of two materials. As the solution is a PDE, this behavior was not desirable (but it was found in the cited literature). A solution for this discontinuity is the use of the Laplace transform (Carslaw, 1986, Viana 2023 and Wanzeller, 2023). In fact, Carslaw makes it clear that discontinuity problems cannot be treated using this mathematical tool.

References

Ascher, M. (1960). Explicit Solutions of the One-Dimensional Heat Equation for a Composite Wall, Mathematics of computation. 14, 346–53.

Bautista-Baños, S., Correa-Pacheco, Z. N., Ventura-Aguilar, R. I., Landa-Salgado, P., Cortés-Higareda, M., & Ramos-García, M. d. L. (2025). Traditional and Recent Alternatives for Controlling Bacterial Foodborne Pathogens in Fresh Horticultural Commodities—A Review. Coatings, 15(5), 597. https://doi.org/10.3390/coatings15050597.

Bedane, T., Di Maio, L., Scarfato, P., Incarnato, L. & Marra, F. (2015). Modeling and sensitivity analysis of mass transfer in active multilayer polymeric film for food applications, AIP Conference Proceedings. 1695, 020062.

Carranza, S., Paul, D. R. & Bonnecaze, R. T. (2012). Multilayer reactive barrier materials. Journal of Membrane Science. 399-400, 73-85. Carslaw, H. S. (1986). Conduction of Heat in Solids, Oxford University Press, USA; 2nd ed.

COMSOL, https://www.comsol.com/.

Di Maio, L., Bedane, T. L., Marra, F., Incarnato, L., & Saguy, S., (2017). Oxygen transfer in co-extruded multilayer active films for food packaging. AIChE Journal. 63(11), 5215–21 (2017).

Ferrari, M. C., Carranza, S., Bonnecaze, R. T., Tung, K. K., Freeman, B. D. & Paul, D. R. (2009). Modeling of oxygen scavenging for improved barrier behavior: Blend films. Journal of Membrane Science. 329(1–2), 183–92.

Gaikwad, K. K., Singh, S. & Lee, Y. S. (2018). Oxygen scavenging films in food packaging. Environ Chem Lett. 6, 523–38.

GRACE, https://plasma-gate.weizmann.ac.il/Grace/.

Iserles, A. (2008). A First Course in the Numerical Analysis of Differential Equations, Cambridge University Press.

Kadirvel, V., Palanisamy, Y. & Ganesan, N. (2025), Active Packaging System—An Overview of Recent Advances for Enhanced Food Quality and Safety. Packag Technol Sci. 38: 145-62. https://doi.org/10.1002/pts.2863.

Keller, P. E. & Kouses, R. T. (2017). Water vapor permeation in plastics, Pacific Northwest National Lab.(PNNL), Richland, WA (United States).

MATLAB, https://www.mathworks.com/products/matlab.html.

Realini, C. B. & Begonya, M. (2014). Active and intelligent packaging systems for a modern society, Meat Science. 98(Issue 3), 404.

Silva, L. G., Wanzeller, W. G. D. & Fernandes, C. A. (2024). Computational modeling of a food packaging using finite elements. Foco (faculdade novo milênio). 17, e4725.

Viana Batista, R., Gonçalves Wanzeller, W. & Menezes, V. M. (2023). Mathematical model and numerical simulation of oxygen transport in multilayer food packaging: a semi-analytical approach. Regionem: Revista Interdisciplinar em Desenvolvimento Sustentável. 1, e12864.

Viana, R. B., Wanzeller, W. G., Lim, L., Pinto, V. Z., Quast, E. & Menezes, V. M. (2022). Food Packaging and its Oxygen Transfer Models in Active Multilayer Structures: A Theoretical Review. Journal of Plastic Film and Sheeting, v. 1. Doi: http://doi.org/10.1177/87560879211070465

Vilas, C., Mauricio-Iglesias, M. & Garcia, M. R. (2020). García, Model-based design of smart active packaging systems with antimicrobial activity, Food Packaging and Shelf Life. 24, 100446. https://doi.org/10.1016/j.fpsl.2019.100446.

Wanzeller, W G, Dagnone, C. A. F. , CAstro, G. M. & Alves, C. (2023). On the use of numerical inverse Laplace transform applied to heat conduction in multilayer materials. The International Journal of Engineering & Science (The IJES) (online). 12, 47-52.

ZENODO, https://zenodo.org/records/3478375 10)