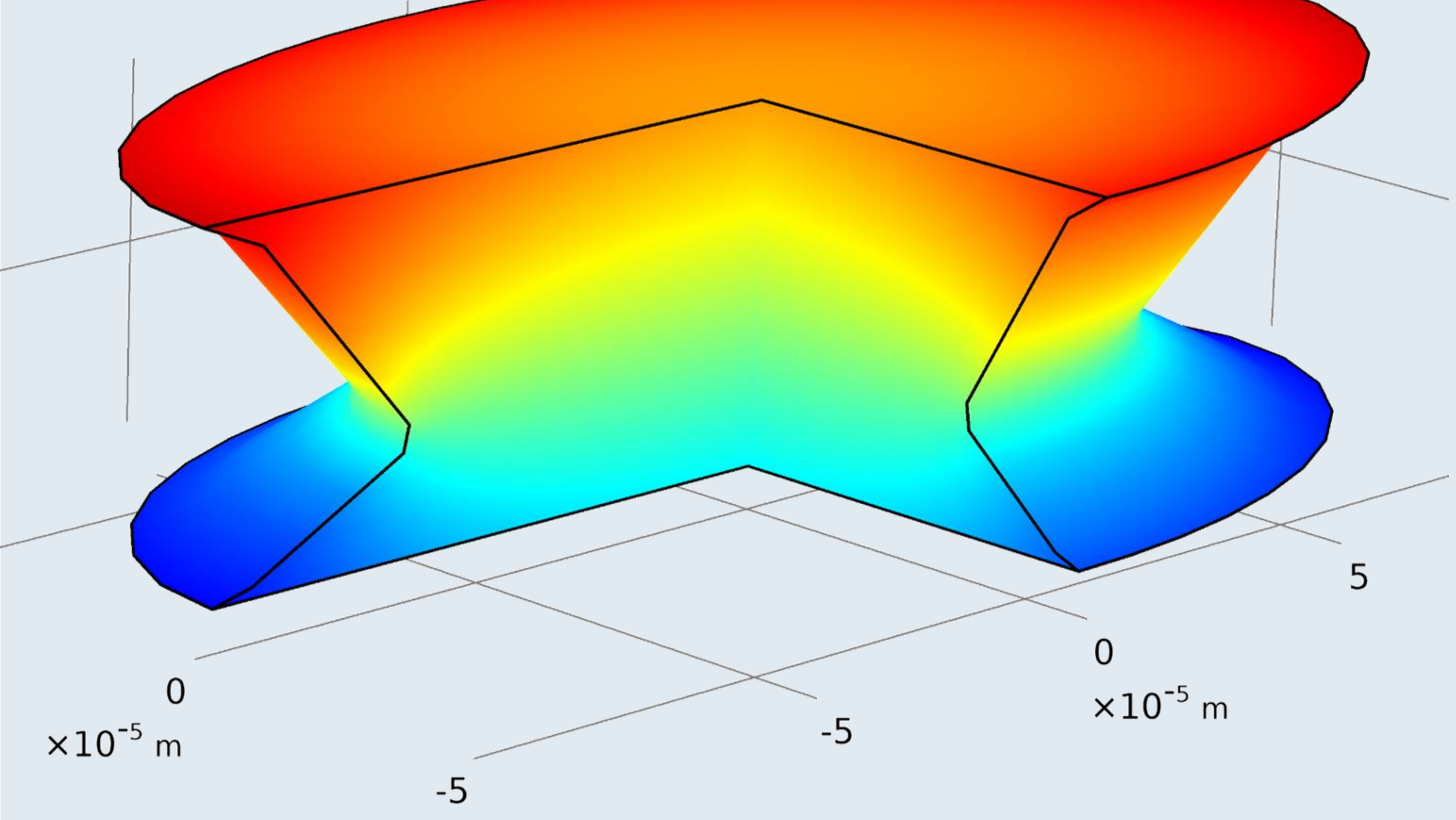

A COMSOL Multiphysics® 3D CFD Model for Describing the Gas Exchange Through Microperforations

The developed approach is a fully coupled model combining the transport of species through the Maxwell-Stefan equations, and laminar flow by Navier-Stokes equations for compressible Newtonian flow, and considers that gas composition as a ternary mixture of of CO_2, N_2 and O_2.

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Introduction and Goals

Modified Atmosphere Packaging (MAP) is a widely applied technology for the shelf-life extension of fresh and fresh-cut fruits and vegetables. This technique relies on modifying the gas composition inside de package by the respiratory activity of the product and the gas exchange through the package. The incorporation of microperforations (holes between 50-300 μm in diameter) in the packages may extend the potential applications of MAP systems, since it may increase the gas exchange and modulate the permselectivity through packages. In the recent years, many researchers have developed models to quantify the gas exchange through perforations and predict the evolution of the gas composition in perforated packages. As the packaging material is usually a polymeric film, the gas exchange through microperforated packages is considered the sum of two mechanisms, permeation through the continuous packaging film and diffusive flow through the perforations, with the latter contributing significantly to the overall flux. However, most of the models do not consider either the convective fluid-dynamic transfer of gas through the perforation or the spatial dependence of the gas concentration in the headspace, although it is a fact that in the surroundings of the perforation the gas concentration differs from that of the rest of the package.

The **objectives** of this work were:

1. **Develop a 3D, spatial-time dependent mathematical model to simulate the gas exchange through a microperforation, considering both convective and diffusive flux.**
2. **Verify the predictions of the gas evolution with the results obtained in an experimental system where fluid dynamics conditions are similar to those generated inside microperforated packages of respiring products.**
3. **Gradually simplify the model to reduce the computation time by creating simpler geometries and equations, while maintaining the accuracy of the predictions.**

EXPERIMENTAL SYSTEM

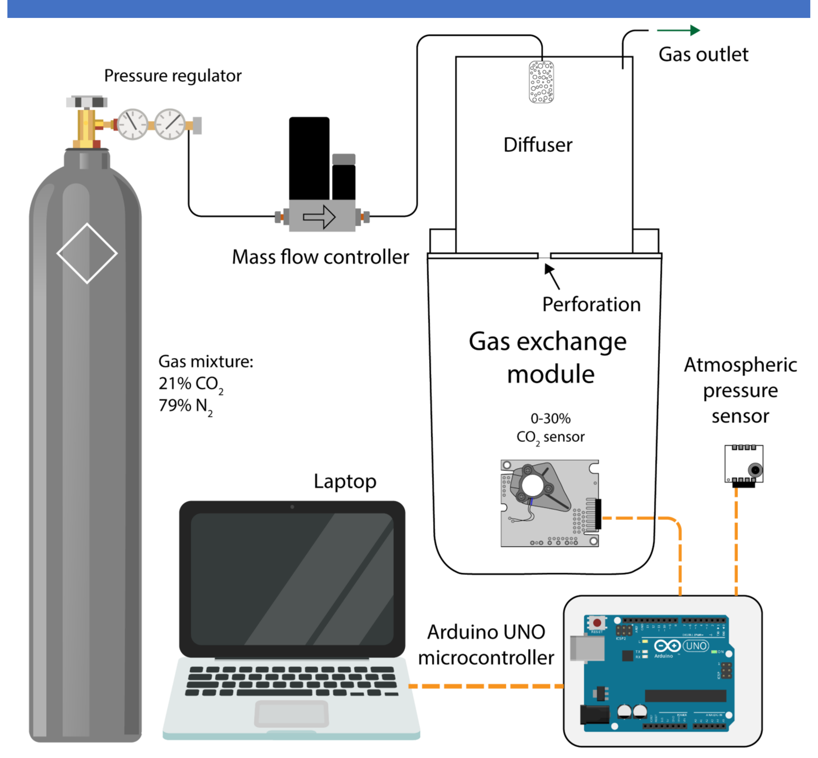

Figure 1. Schematic diagram of the experimental system built to measure the CO2 exchange through a microperforation and the changes in atmospheric pressure.

3D COMPUTATIONAL MODEL

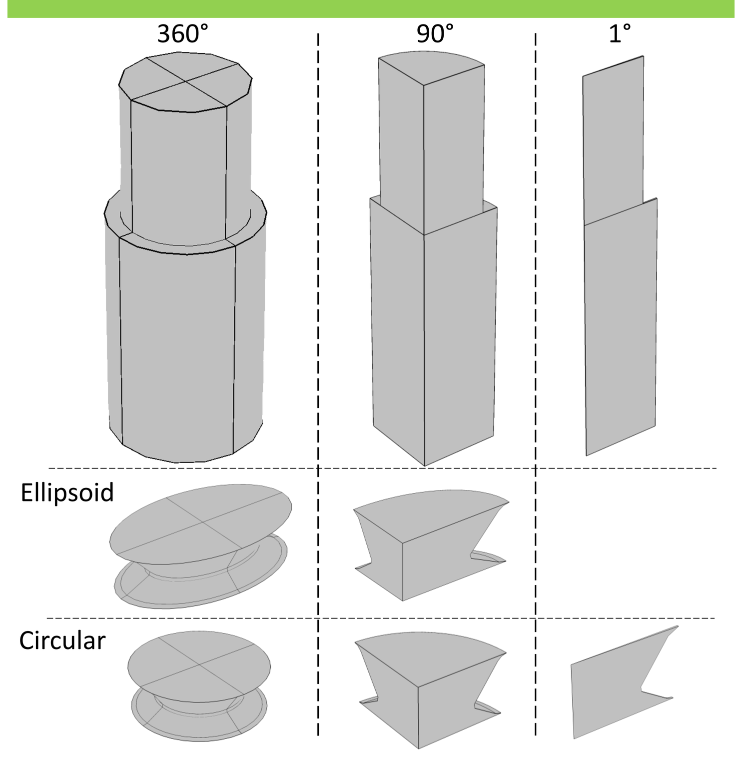

Figure 3. Computational domains.

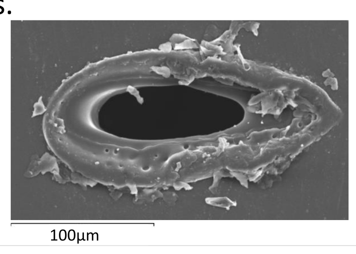

Figure 2. Scanning electron microscope image of the microperforation.

Materials and Methods

The experimental system, based on the design by González-Buesa and Salvador (2022) (Figure 1), was able to measure the gas transmission rate through microperforations. The system comprises two chambers: the upper chamber containing a mixture of 21% CO_2 and 79% N_2, and the lower chamber (1.25L) initially filled with atmospheric air. These chambers are separated by a lid where the microperforations is located. In the lower chamber, a CO_2 sensor (k33 ICB 30%, Senseair, Sweden) was installed. Additionally, the experimental system was equipped with an absolute pressure sensor (AMS-5915-1200-B, Analog Microelectronics, Germany) to monitor slight variations in atmospheric pressure. All sensors were controlled using an Arduino UNO (Arduino, Italy). The perforations were chosen from a 50μm-thick film (PPlus 52LD160, Amcor, UK), and were measured using a microscope at 20X (Axio Scope A1 AX10, Carl Zeiss Microscopy GmbH, Germany). Perforations were observed from above (Figure 2), and the measured area corresponds to those of the minimal dimensions. The selected perforations had an average size of 7460.65 μm^2.

The gas exchange through a perforation was treated as a coupled transient mass and momentum transfer phenomenon. Mass transport included convection and diffusion, with the mass fractions of various gases describing using the Maxwell-Stefan equations. The momentum transport was characterized by the Navier-Stokes equations for compressible Newtonian flow.

In this study, the described physics were implemented in a 3D computational model using COMSOL Multiphysics® (Figure 3). The specific module utilized was Chemical Reaction Engineering, with a focus on the Transport of Concentrated Species and Laminar Flow, enabling the creation of a Multiphysics system. Three domains were established: the upper chamber, the lower chamber, and the perforation path. The boundary conditions were set as follows: symmetry applied to the internal faces, an inlet of a gas mixture consisting of 0,2095 CO_2, 0,0005 O_2 and 0.79 N_2 on the upper face of the upper chamber, and outlet on the lateral external face with barometric pressure conditions outside, impermeability in all other cases, and continuity between the domains. To solve this model, PARDISO was employed, with a total simulation of 216 hours, a time step of 30 seconds, and a solution save interval of 1 hour. Several simplifications in system's geometry, physics, or meshing were introduced in the model, as shown in Table 1.

Table 1. Conditions of the six proposed models.

System's geometry	Physics	Pressure	Perforation's geometry	DOFs	Mesh					
					Element Size			Mesh elements	Quality	
					Calibrate	Perforation	Remaining		Minimum	Average
360°	Maxwell-Stefan	Atmospheric	Ellipsoid	171208	Fluid dynamics	Extra Fine	Extra coarse	33844	0.1491	0.6509
360°	Maxwell-Stefan	Atmospheric	Circular	177932	Fluid dynamics	Extra Fine	Extra coarse	35139	0.1792	0.6521
360°	Maxwell-Stefan	Constant	Circular	177932	Fluid dynamics	Extra Fine	Extra coarse	35139	0.1792	0.6521
360°	Fick's law	Constant	Circular	177932	Fluid dynamics	Extra Fine	Extra coarse	35139	0.1792	0.6521
90°	Maxwell-Stefan	Constant	Circular	184915	Fluid dynamics	Coarser	Coarser	35789	0.0574	0.6606
1°	Maxwell-Stefan	Constant	Circular	135566	General physics	Finer	Fine	17065	0.0049	0.1609

Results

The evolution of CO_2 concentration recorded in the experimental system was compared with that obtained from numerical simulation (Figure 4). Apparently, the computational results are similar, so these data do not provide the necessary information to determine which model is the most suitable for accurate prediction of gas transport though microperforations using the shortest calculation time. The more complex model accurately predicted gas exchange though the microperforation but entailed significant computational costs. Therefore, the computational time and the Root Mean Squared Error (RMSE) over experimental data were compared for each of the simplifications proposed in the models (Figure 5).

In part a), the results of transforming the perforation geometry from elliptical to circular while preserving the same area are presented. No significant differences in simulation time and RMSE are observed between both cases, indicating that this simplification has little impact on the model. The comparison of simulations conducted with atmospheric pressure input and with constant pressure is illustrated in part b). In this case, computational time for simulations with atmospheric pressure is significantly higher because, to obtain error-free results, it was necessary to select specific conditions for the study. Adjustment to the method and termination criteria were required, including changing the Jacobian update to occur at every iteration rather than minimally. Additionally, the maximum number of iterations was increased from 4 to 25, and the tolerance factor was reduced from 1 to 0.1. These changes in models using atmospheric pressure were necessary due to the pronounced variation in pressure. The use of Maxwell-Stefan equations or Fick's law to describe the physics of the system (part c) hardly affects accuracy. In addition, the computation time using Fick's law was not reduced as could be expected because it is a simpler equation. The final comparison aimed to simplify the system's geometry (part d). Due to rotational symmetry, it became possible to simulate narrow regions of 90° or 1°. These cases were performed with circular geometry for the perforation because it is not feasible to simulate an ellipsoid by rotation of a 1° region.

In summary, all the proposed models accurately describe gas exchange through microperforations (RMSE<0.5 %). Considering constant pressure instead of variable pressure according to atmospheric conditions is the case, among those studied, that most reduces the computation time. Furthermore, the results reveal that it is no necessary to simulate the whole physical system since considering only a 1° region does not reduce the accuracy. For future modifications of the model involving more variables and complexity, simulating with a 1° geometry will be feasible, as it results in a simpler matrix.

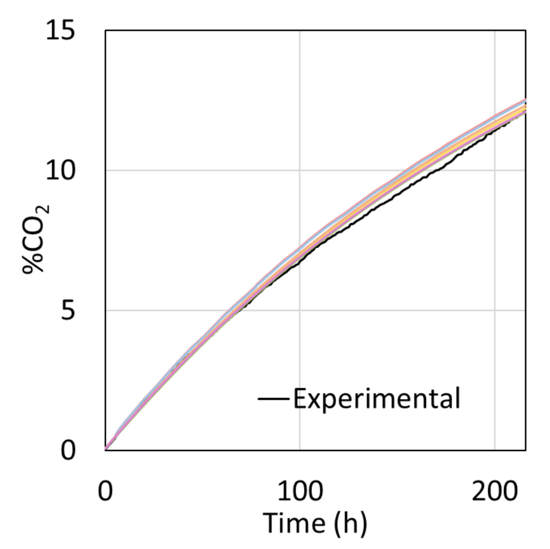

Figure 4: Evolution of CO_2 concentration: black line corresponds to experimental data, and coloured lines correspond to computational results of the different proposed models (Table 1).

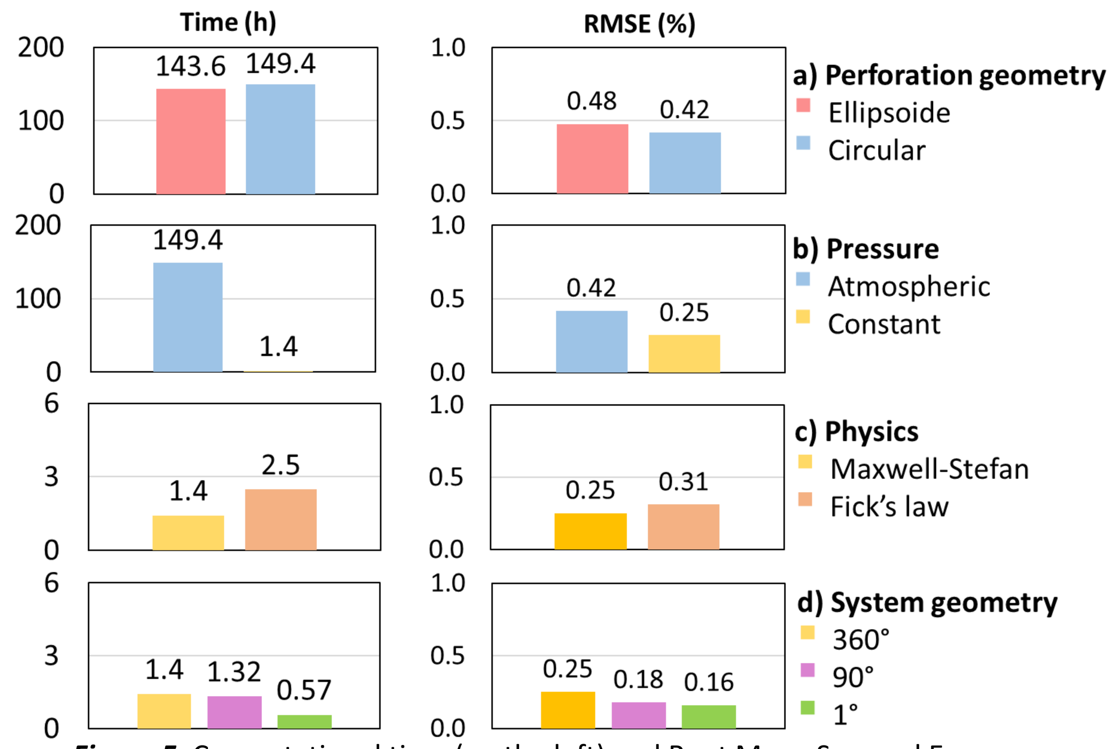

Figure 5: Computational time (on the left) and Root Mean Squared Error, RMSE (on the right) for the different models.

REFERENCES

González-Buesa, J., and Salvador, M.L. (2022). A multiphysics approach for modeling gas exchange in microperforated films for modified atmosphere packaging of respiring products. Food Packag. Shelf Life, *31*.

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