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Coupled CFD-Structural Mechanics Simulation Of Deformation In Non-Rigid Polypropylene Food Packaging

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Abstract

Understanding deformation in non-rigid food packaging is critical for ensuring product safety during processes involving pressurization such as sterilization. Polypropylene (PP) trays sealed with thin lidding films are especially vulnerable to rupture at the heat-seal zone under internal pressure buildup. This study focuses on predicting film displacement during controlled air injection into PP trays using a coupled Computational Fluid Dynamics (CFD) and Structural Mechanics approach. A 2D model of an empty PP tray was developed in COMSOL® Multiphysics 6.3 to simulate airflow and film deformation under inlet flow rates of 0.10, 0.15, and 0.60 L/min. The model reproduced the experimental displacement of the PP film with a normalized root mean square error (RMSE) of 8.52% and predicted the maximum displacement of PP film in the range of 8–11 mm, which is in close agreement with the experimental value of around 10 mm. This study provides a simplified fluid structure interaction model dedicated to prediction of PP film deformation under pressurized air. The model highlights the role of displacement thresholds of PP packaging film under pressurization.

Keywords: Computational fluid dynamics (CFD), structural mechanics, numerical modelling, simulation, food packaging

Introduction

Food packaging plays a central role in ensuring the safety, quality, and shelf life of thermally processed products. During sterilization or other high-pressure treatments, internal pressure builds up inside the packaging due to gas expansion and vapor generation, exerting significant mechanical stress on the sealing film and flange region of packaging trays. This can lead to deformation and, rupture of the packaging, compromising both product safety and consumer confidence. Non-rigid packaging systems such as polypropylene (PP) trays sealed with thin polymer films are particularly vulnerable because their structural integrity depends strongly on the sealing interface rather than the bulk material strength.

Earlier studies have shown that rupture of PP trays occurs at the heat-seal interface, which is the weakest zone of the package [1]. Pressure accumulation inside the tray is sufficient to deform the lidding film until it detaches or tears at the sealing edges. The risk of rupture increases with higher pressure differentials. Hence, there is the need to understand how internal pressurization translates into film deformation and seal failure. In practice, industrial processes attempt to mitigate this risk by controlling external counter-pressure, but a quantitative understanding of the fluid–structure interactions inside the package remains limited.

Computational modelling offers a powerful approach to study these coupled phenomena [2], [3]. In previous work, pressure evolution inside rigid containers was examined [4]. Whereas much less attention has been given to non-rigid polymeric trays where deformation is a critical aspect of package performance. In particular, little is known about the influence of pressurization on film displacement and the onset of rupture. Numerical models that couple Computational Fluid Dynamics (CFD) with Structural Mechanics can provide valuable insights by simultaneously predicting the internal pressure buildup and the deformation of the sealing film under transient loading.

The objective of this study is therefore to develop and validate a coupled CFD–structural mechanics model to simulate the deformation of PP trays during controlled air injection. The focus is placed on a simplified 2D configuration representing an empty tray subjected to constant inlet air flowrates. Experimental data on film displacement are used to validate the model. Moreover simulated internal pressure values are also reported. This work represents a first step towards establishing predictive tools for packaging integrity, which can later be extended to include thermal effects, vapor

generation, and 3D geometries relevant to heat treatment processes.

Experimental Setup

The experimental study was carried out using commercially available polypropylene (PP) trays (Figure 1), which are commonly used for ready-to-eat meals. Each tray was sealed with a PP lidding film of around 65 µm thickness using an industrial sealing system (Multivac, Type Galaxy, TS 355) at 160°C and available at Oniris-Nantes, France. For the present work, the trays were kept empty. During the experiments, air was injected into the trays through a small stainless-steel inlet tube that was fitted at one side of the tray. The air supply was regulated using a mass flow controller to deliver constant air flow rates. Three flow conditions were studied: Q1: 0.10, Q2: 0.15, and Q3: 0.60 L/min. The absolute internal pressure inside the trays was measured using pressure sensors (NanoVACQ PT, TMI-Orion, France). At the same time, a high resolution digital camera (Go, JAI Ltd., Japan) positioned horizontally to the tray captured images at one frame per second in order to record the progressive displacement of the film. The vertical dome height at the center of the tray was later extracted from these images by means of an image analysis software, ImageJ [5]

Rupture of the system was identified by a visible rupture of the PP film close to the heat-seal region in the recorded images. For each airflow condition, the maximum film displacement was determined. Figure 2 displays the experimental setup of the air injection system consisting of air inlet tube, background light, and high definition digital camera.

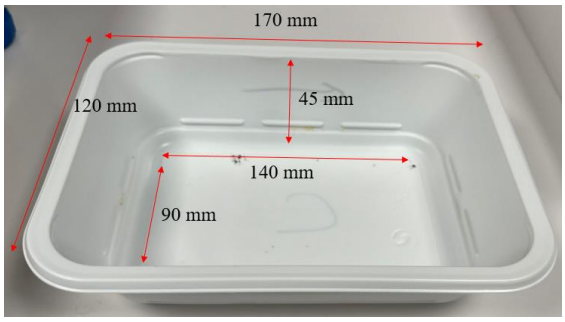

Figure 1: Image of the PP tray with dimensions.

Numerical Model

A numerical model was developed using COMSOL® Multiphysics 6.3 software by employing the CFD and Solid Mechanics modules. The internal airflow (laminar) (Reynolds number of 47.38, 71.07, and 284.29 for Q1, Q2, and Q3 respectively) was simulated using the compressible Navier-Stokes equations (time-dependent study), and the structural mechanics of the PP film was modeled using equations for deformable solids (time-dependent study). The coupled solution of these physics allowed the simulation of fluid–structure interaction (FSI) between the injected air and the PP film.

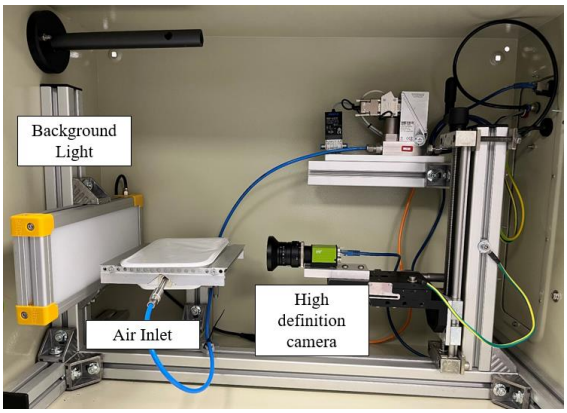

Figure 2: Experimental setup of the air injection system.

Governing equations
Computational Fluid Dynamics (CFD):

The airflow inside the tray was described using the compressible Navier–Stokes and continuity equations [6]:

$$\rho\frac{\partial \boldsymbol{u}}{\partial t}+\rho(\boldsymbol{u}.\nabla)\boldsymbol{u}=\nabla.[-p\boldsymbol{I}+\boldsymbol{K}]+\boldsymbol{F} \quad (1)$$

Conservation of mass was ensured by solving the continuity equation [7]:

$$\frac{\partial \rho}{\partial t}+\nabla.(\rho\mathbf{u})=0 \quad (2)$$

Structural Mechanics and Fluid-Structure Interactions

The conservation of momentum for a deformable solid is expressed as [8]:

$$\rho\frac{\partial^2 \boldsymbol{u_s}}{\partial t^2}=\nabla.S+\boldsymbol{F}_v \quad (3)$$

where ρ is the density of the solid (kg/m^3), $\boldsymbol{u_s}$ is the displacement vector (m), S the second Piola–Kirchhoff stress tensor, and $\boldsymbol{F}_v$ is the body force per unit volume (N/m^3).

Initial conditions

The initial air velocity field was defined as

$$u_0=0\ m/s \quad (4)$$

The initial relative pressure inside the PP tray was taken as

$$p_0 = 0\ Pa \tag{5}$$

The initial displacement of the PP film was set to

$$\boldsymbol{u_s} = \begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix} m \tag{6}$$

Boundary conditions

The inlet boundary condition was prescribed as a mass flow. The injected air entered the tray at the defined flow rate:

$$\int \rho(\boldsymbol{u}.\boldsymbol{n})dS = \dot{m} \tag{7}$$

$$\dot{m} = \rho Q_i \tag{8}$$

The inlet volumetric flow rates were applied as three cases of Q_i: $Q_1 = 0.10\ L/min$; $Q_2 = 0.15\ L/min$; $Q_3 = 0.60\ L/min$

On all tray walls, the no-slip condition was imposed to set the fluid velocity to zero:

$$\boldsymbol{u} = \begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix} m/s \tag{9}$$

The tray body and film edges were fixed to prevent rigid-body motion:

$$\boldsymbol{u_s} = \begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix} m \tag{10}$$

The fluid pressure acted on the structural surface of the PP film as a traction load, expressed as a film load of pressure:

$$\delta W = \int [(-p\boldsymbol{n}) \cdot \delta \boldsymbol{u}]dA \tag{11}$$

This is used to couple fluid pressure to structural deformation. δW is the pressure-volume work associated with fluid motion that acts on the PP film. A is the surface area of the PP film over which the pressure acts in upward direction.

Model description

A 2D model of the empty PP tray (filled with air) was chosen in COMSOL® Multiphysics 6.3 (Figure 3) as a first approximation to reproduce the experimental configuration. The geometry included the fluid domain representing the injected air inside the tray and the boundary representing the PP film and PP tray. A small inlet was defined at one left side of the tray to impose the airflow boundary condition (same value as for experimental setup). The air domain was modeled as compressible laminar flow. The PP film was modeled as a linear elastic material.

Thermophysical properties of air at 20°C were imported from the COMSOL® material library, while the mechanical properties of the PP film (Young's modulus and Poisson ratio) were obtained from literatures and parametrically fitted (results not reported) against experimental data. The best-fit mechanical properties used in this study were a Young's modulus of 1.847 GPa and a Poisson ratio of 0.42 as reported in literatures [12]. Table 1 lists the input parameters for the model. A user-controlled mesh was applied with a total of 3190 triangular elements. The study was computed for a time range of 0 to 100 s for all three inlet flow rates (0.10, 0.15, and 0.60 L/min).

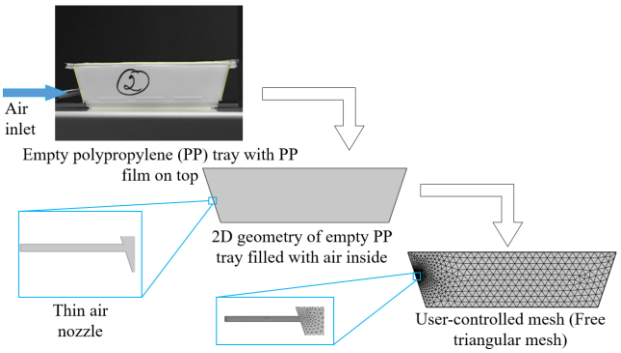

Figure 3: Polypropylene (PP) food tray with PP film on top and meshing in COMSOL® Multiphysics 6.3.

Table 1: Input Model Parameters

Parameters	Values	References
Density of PP	930 kg/m^3	[9]
Thickness of PP film layer	6.5 × 10^{-5} m	measured

Simulation Results

The numerical model was computed for a total duration of 100 s for all three inlet flow rates. The results obtained from the simulations were compared with experimental data collected from the air injection experiments to assess the accuracy and reliability of the numerical methods.

Film displacement

The experimental PP film displacement profiles were compared with the simulated displacement under all the three different flow rates (Figure 4). The simulated profiles reproduced the experimental trends, showing gradual dome growth at low flow rates and faster deformation at higher flows.

At a flow rate of 0.10 L/min, the model predicted a maximum dome displacement of 8.66 mm at 94 s, compared to the experimental value of 10.00 ± 1.05 mm. At 0.15 L/min, the simulated displacement reached 10.18 mm at 83 s, close to the experimental

value of 10.80 ± 0.27 mm. For the highest flow rate of 0.60 L/min, the simulation produced a displacement of 11.24 mm at 25 s, compared to the experimental value of 10.70 ± 0.30 mm. The measurement of all the experimental values were performed with an image precision of 1 mm = 11.644 pixels. The model predicted the PP film displacement with a normalized RMSE of 8.52%. Figure 5 shows the experimental displacement images and 2D simulated displacement of PP film at the time of rupture with different air flow rates.

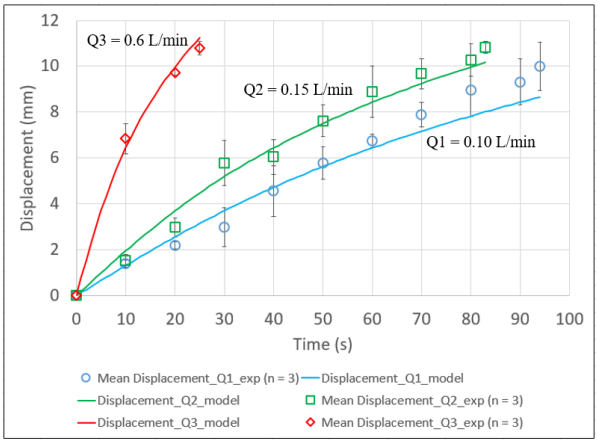

Figure 4: Simulated and experimental displacement values of PP film from original position with respect to different air flowrates (0.1 L/min, 0.15 L/min, 0.6 L/min). Number of repetitions, n = 3.

Pressure modelling

The experimental pressure profiles inside the tray were compared with the simulated pressure profiles obtained from the coupled CFD and structural mechanics model. Figure 6 presents the comparison between simulated and experimental relative pressures at the three inlet flow rates. The model simulated that the internal pressure inside the tray rose faster as the air flowrate increased from 0.10 to 0.60 L/min. The simulated maximum pressure was reported as 41 mbar (compared to 42 mbar experimental maximum pressure) for 0.10 L/min, 41 mbar (compared to 41 mbar experimental maximum pressure) for 0.15 L/min , and 45 mbar (compared to 46 mbar experimental maximum pressure) for 0.60 L/min. However, validation is necessary with more experimental trials for this pressure model.

Discussions

The coupled CFD–structural mechanics model developed in this study reproduced the experimental trends obtained from image analysis for the PP film displacement.

The internal pressure during air injection was also simulated but it still needs more number of experimental repetitions to validate the pressure prediction model as a single repetition is not sufficient.

The model captured the essential physics of tray deformation under air injection. The simulations confirmed that as air enters the tray, pressure builds up in the tray and inflates the PP film at the center. The onset of rupture was consistently associated with film displacements of approximately 8–11 mm, in line with experimental observations (approx. 10 mm). At these displacements, the model predicted that the tray could sustain a maximum pressure of less than 50 mbar. This is in line with the experiments with one repetition where the maximum pressure before rupture was measured around 45 mbar. The rapid higher pressure observed at Q3 compared with Q1 and Q2 is due to the larger mass flow rate of injected air, which increases the number of air molecules entering the tray per unit time. As the tray volume remains constant, this greater influx accelerates pressurization, leading to a steeper pressure rise, which in turn leads to faster PP film displacements. This 2D approach captures the main deformation behavior but it cannot account for three-dimensional effects such as corner stresses and seal-zone behavior.

The deformation of the PP film is a direct response to the buildup of air pressure inside the tray. As air was injected, the rise in internal pressure created an outward force on the film, leading to progressive displacement at the tray center where the load was distributed. The model predicted PP film displacement with good agreement to experiments because the mechanical properties of the PP film (Young's modulus and Poisson ratio) were preliminary fitted to match the observed deformation. Further investigation is required to understand the stress distribution on the PP film during this pressurization with air injection.

Conclusions

A 2D CFD–structural mechanics model was developed in COMSOL® Multiphysics 6.3 to study the deformation of polypropylene (PP) food trays during controlled air injection. The model coupled compressible laminar airflow in the headspace with the elastic deformation of the PP lidding film, and was validated against experimental measurements of film displacement at three air flow rates.

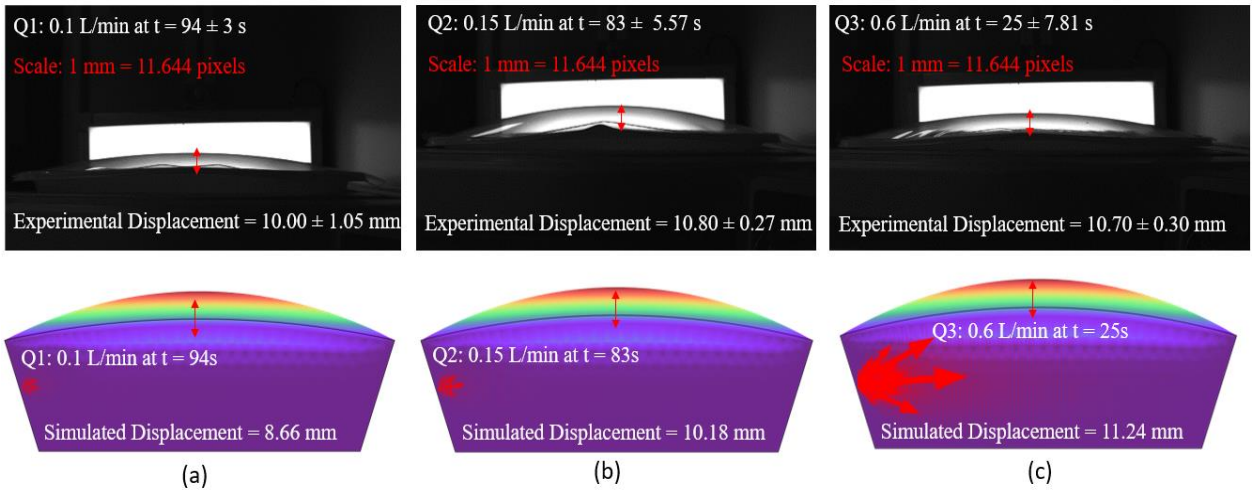

Figure 5: Experimental displacement images and 2D simulated displacement images of PP film at the time of rupture with different air flow rates (a) Q1: 0.1 L/min at t = 94 s (b) Q2: 0.15 L/min at t = 83 s (c) Q3: 0.6 L/min at t = 25 s. The simulated displacement values of PP film are scaled.

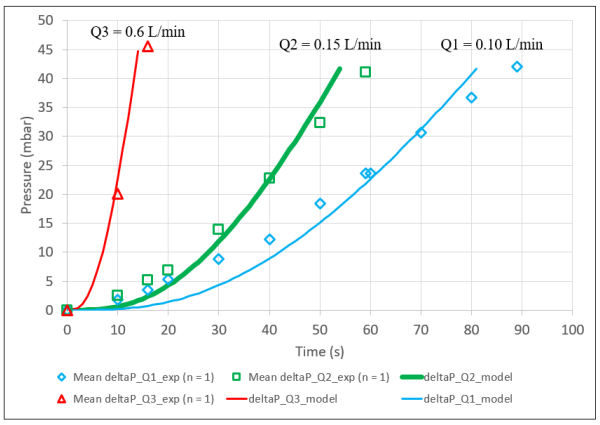

Figure 6: Simulated relative pressure (deltaP) values inside PP tray different air flowrates (0.1 L/min, 0.15 L/min, 0.6 L/min).

The simulations reproduced the experimental results with maximum displacement values closely matching experimental image analysis (normalized RMSE of 8.52%). The model also simulates the internal maximum pressure. However, the pressure model remains to be validated with additional number of experiments. Greater importance was given to the study of PP film displacement in this study, as the main objective was to determine the maximum deformation the film can undergo for given mechanical properties of PP (Young's modulus and Poisson ratio) and to compare these values directly with experiments. As a result, displacement served as the most robust parameter for validating the model.

The main limitations of the study lie in the use of a two-dimensional model, which cannot resolve three-dimensional effects such as corner stresses. Moreover, rupture was not directly predicted as a material failure in the model but inferred from the displacement threshold observed experimentally. In reality, rupture originates at the heat-seal interface through complex adhesive and cohesive failure mechanisms that were not represented in the present simulations.

Despite these limitations, the present work represents an important first step in quantitatively linking air flowrate and deformation in non-rigid polypropylene packaging. The 2D CFD–structural mechanics framework developed here provides a baseline model that can be extended to more complex conditions. Further studies should thus focus on investigating the air flow patterns with a 3D model to understand the fluid-structure interactions leading to the rupture of packaging.

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Acknowledgments

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