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Improving the Oxygen Removal Process in a Chamber Using Computational Fluid Dynamics Simulations for Pest Control Applications

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Abstract: This study focuses on post-harvest pest management in agriculture, in particular the transition to modified atmospheres as a sustainable alternative to conventional pesticide methods. Using Computational Fluid Dynamics (CFD) simulations, we analysed the dynamics of oxygen distribution within a pest control chamber. We tested four different configurations of nitrogen inlet and outlet positions to determine the most effective setup. The simulations used the twoLiquidMixingFoam solver in OpenFOAM to model gas mixing and diffusion. Our results show that the configuration with the nitrogen inlet at the top and the outlet at the bottom (Case D) was the most efficient. This configuration reached the target oxygen concentration of 1.5% in 4.4 h, significantly faster than the other configurations. These results highlight the importance of inlet and outlet positioning in improving the efficiency of oxygen reduction and ensuring a consistent low oxygen level throughout the chamber. Optimising the placement of nitrogen inlets and outlets has significant potential to improve the effectiveness of modified atmosphere treatments for pest control. Future research should consider additional environmental factors, different storage conditions and insect mortality models to further refine these methods.

Keywords: computational fluid dynamics; simulation; nitrogen; modified atmospheres; low oxygen; insects; stored product protection

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1. Introduction

Modified atmospheres present a promising solution for managing insects during the post-harvest stages of agricultural products (cereals, dried fruits, nuts, etc), offering a viable alternative to conventional pesticides. With increasing consumer concerns about the hazards of residual insecticides in food and their harmful environmental impacts, the adoption of modified atmospheres on an industrial scale is emerging as a feasible and eco-friendly pest control strategy for various commodities [1–3].

The term "modified atmospheres" refers to techniques that alter the proportions of gases within a specific space, such as a chamber. This process typically involves the introduction of gases like nitrogen or carbon dioxide to substantially reduce oxygen levels or increase carbon dioxide concentrations [3,4]. This deliberate modification of the atmosphere exploits the dependence of insects and many microorganisms on oxygen for their aerobic processes, thereby severely hindering their development and survival [3,5].

The benefits of using modified and controlled atmospheres for disinfestation are numerous. Primarily, these methods are environmentally friendly and significantly reduce the use of chemical pesticides, thereby minimizing pesticide residues in stored products [6]. This approach aligns with the increasing consumer demand for safer and more sustainable agricultural practices. Additionally, modified and controlled atmospheres are non-toxic to humans, posing no health risks to workers or consumers [7]. They also mitigate the risk of pests developing resistance, a major issue with traditional chemical treatments [8,9]. Consequently, these methods can be incorporated into integrated pest management (IPM) strategies, supporting long-term pest control and reducing the necessity for repeated treatments [9].

In spite of the advantages of modified and controlled atmospheres, phosphine fumigation remains the predominant method for pest control due to its straightforward application process (requiring a sealed environment and appropriate dosage) and lower operational costs (primarily associated with fumigant purchase and application labor) compared to controlled atmospheres [10]. Controlled atmospheres incur higher installation costs due to the need for specialized equipment like nitrogen generators, gas distribution systems, and airtight storage chambers. One potential financial advantage of controlled atmospheres could be realized through logistical efficiencies, particularly in reducing treatment durations [4]. Phosphine fumigations typically last between 4 to 12 days (according to the Coresta protocol [11]), depending on factors such as temperature, phosphine concentration, targeted insect species, and treated commodity. Similarly, scientific studies suggest exposure durations of 2.5 to 9 days for nitrogen treatments in low oxygen atmospheres, depending on temperature and insect species [12,13]. To capitalize on these shorter exposure periods, it is crucial to design chambers that rapidly achieve desired low oxygen levels without adding unnecessary delays to the process, which is the primary objective of this study.

Despite the promise of using modified atmospheres with nitrogen and the growing body of research on insect responses to low-oxygen environments, there is limited information on the optimal configuration of nitrogen inlets and outlet positions and their impact on treatment times, as highlighted in the following references of relevant scientific studies. Numerical investigations provide a valuable approach, allowing storage managers and practitioners to gain a deeper understanding of the fundamental mechanisms governing nitrogen and oxygen diffusion in various storage environments and agricultural commodities. In this context, numerical modelling has been partially applied in similar applications, highlighting its potential to optimize these processes.

Specifically, Agrafioti et al. [12] explored the practical application of modified atmospheres to address phosphine-resistant insect populations in commercial settings. Their study focused on the efficacy of this method against two prevalent species of stored-product beetles, *R. dominica* and *O. surinamesis*. They developed a computational model to assess nitrogen concentration within the commodities (currants) by solving the gas diffusion equation, utilizing known nitrogen/oxygen concentrations in the chamber derived from previous experimental data.

Similarly, Kaloudis et al. [14] employed computational simulations, specifically using the convection–diffusion equation, to examine nitrogen penetration and distribution within two common storage configurations: chamber-contained pallets and silos. Their study investigated the penetration of nitrogen in various agricultural products. For the chamber scenarios, they considered two boundary conditions for oxygen concentration: one with pallets placed in a chamber maintaining a uniform 0.5% oxygen concentration, and another with a gradual decrease in oxygen concentration from atmospheric levels to 0.5%. However, their study did not evaluate the optimal positions for the nitrogen inlet and chamber outlet.

These studies [12,14] were carried out in commercial facilities, utilizing a nitrogen generator to introduce nitrogen into the environment. Each testing chamber contained three to four pallets loaded with either currants or herbs. To evaluate nitrogen concentration, a computational model was developed. This model operated under the assumption that nitrogen concentration remained uniform in the vicinity of the pallets and that gas diffusion was the predominant mechanism of nitrogen dispersion within the pallets. Accordingly, the model solved the diffusion equation. The simulation outcomes revealed that nitrogen could effectively permeate the currants, with minimal concentration discrepancies (less than 1.5%) observed across the pallet. Moreover, the model demonstrated that lower temperatures had an insignificant effect on nitrogen concentration profiles.

Guo et al. [15] conducted a study presenting numerical simulation results on the injection of liquid nitrogen into a container, demonstrating the effectiveness and practicality of controlled atmosphere treatments for preserving mature pepino fruit quality. Their investigation specifically examines the impact of recirculation velocity on oxygen volume fraction and temperature distribution within a controlled atmosphere container following the introduction of liquid nitrogen. They developed a sophisticated three-dimensional (3-D) model and utilized numerical simulations to analyse the airflow, heat transfer, and mass transfer dynamics associated with liquid nitrogen injection. Employing the finite volume method, they solved the governing equations governing mass, momentum, and heat transfer, along with their corresponding boundary conditions. The results of this study provide a comprehensive understanding of air transport in a container. However, they cannot be applied to pest control applications due to differences in inlet and outlet configurations, the lack of investigation into various configurations, and the focus on controlling temperature in addition to lowering oxygen levels.

In a parallel study, Silva et al. [16] conducted research using a computational fluid dynamics (CFD) model to explore the dynamics of ozone gas flow within an aeration system, targeting a lethal concentration for the maize weevil, *Sitophilus zeamais* Motschulsky (Coleoptera: Curculionidae) in rice grains. Leveraging the CFD technique, they modelled gas flow dynamics and calibrated the model to experimental data, considering critical parameters like the mass transfer coefficient and the ozone-rice grain reaction constant. Subsequently, they simulated the injection of ozone gas into a silo with a static capacity of 69.6 tons of rice. Similarly, Carvalho et al. [17] studied nitrogen gas concentration for refrigeration and atmosphere adjustment in corn storage. Additionally, Pandiselvam et al. [18] utilized numerical simulations to forecast ozone concentration and flow characteristics in bulked paddy rice. Moreover, Agrafioti et al. [19] employed CFD to model phosphine gas distribution within grain silos and metal containers, successfully validating this model in real-world scenarios.

Given the above, it is evident that there is a lack of scientific studies on the efficiency and optimization of the initial phase of controlled atmosphere treatments, specifically the oxygen removal process. These optimizations include assessing the optimal positioning of chamber inlets and outlets. Existing computational models in the literature solve the diffusion equation rather than the Navier-Stokes equations. As a result, they can only simulate the controlled atmosphere treatment after the desired low oxygen concentration is achieved, not during the initial phase. Therefore, the primary objective of this study is to evaluate the effectiveness of various oxygen reduction processes and configurations, ultimately proposing optimised protocols for improved pest management practices. Specifically, this study utilizes CFD simulations to determine the optimal locations for the nitrogen gas inlet and the chamber outlet to minimize the time required to achieve the desired reduced oxygen levels. By identifying these optimal configurations, the aim is to improve the efficiency and practicality of using modified atmospheres for post-harvest pest management, contributing to more sustainable and effective agricultural practices. The hypothesis of this research is that the strategic placement of nitrogen inlets and outlets will significantly affect the efficiency of oxygen displacement, thereby influencing the overall effectiveness of the pest control process. However, the complexity of this topic limits the study, making it impractical to cover all scenarios comprehensively. Future research should address factors such as temperature, humidity, pressure variations, different boundary conditions, agricultural products, and storage structures. Including insect mortality models in future studies could provide valuable insights, particularly in understanding the relationship between oxygen distribution and insect control, especially in critical areas like the core of the grain bulk.

2. Materials and Methods

2.1. Chamber Characteristics

To evaluate the positions of the nitrogen gas inlet and outlet, a chamber configuration was selected from the study by Sakka et al. [20], which is representative of typical industrial conditions. The chamber used in this study has the following dimensions: a length of 17 m, a width of 3.95 m, and a height of 2.90 m (Figure 1).

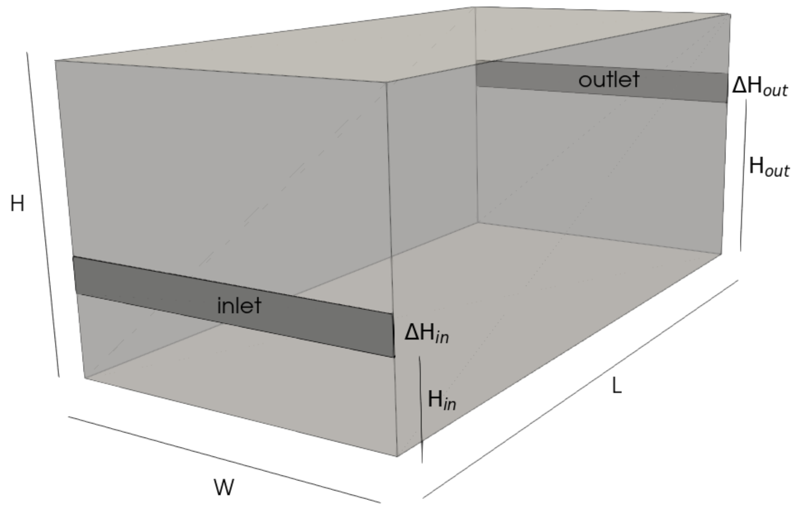

Figure 1. A typical chamber for controlled atmosphere applications. The nitrogen gas is inserted from the front end of the chamber and the outlet is positioned in the rear end. For the present study the height positions of inlet and outlet are under investigation.

Nitrogen was introduced into the chamber through an integrated nitrogen generator (Ali 4100). Both the inlet and outlet for the nitrogen have openings of 0.2 m in height. High purity nitrogen (comprising 99.0% N_2 and 1.0% O_2) was generated from ambient air using a pressure swing adsorption (PSA) process. This nitrogen was then pumped into the chamber at a maximum flow rate of 72 cubic meters per hour $[m^3/h]$, ensuring a consistent and controlled introduction of the gas. Thus in an ideal process, after the duration of one fill time (2.7 h), which is the time to fill the entire chamber with nitrogen if no diffusion would occur, the entire chamber should reach 1.0% O_2. The primary focus of this study is to evaluate the impact of varying the heights position of the nitrogen inlet and outlet on the efficiency of oxygen reduction within the chamber. By conducting numerical simulations, we aim to identify the optimal configuration that achieves the target oxygen concentration of 1.5% O_2 in the shortest possible time. Four different scenarios were simulated in this study, involving all combinations of the inlet and outlet positions being either at the bottom (H_{in} or H_{out} = 0 m) or the top (H_{in} or H_{out} = 2.7 m) of the chamber (Table 1). Through this approach, we seek to provide valuable insights and recommendations for optimizing the design and operation of controlled atmosphere chambers, enhancing their effectiveness in post-harvest pest management applications.

Table 1. Location of the inlet and outlet for each case studied.

Case	Inlet Location	Outlet Location
A	bottom	top
B	bottom	bottom
C	top	top
D	top	bottom

2.2. Computational Model Description

Numerical simulations were performed with the OpenFoam CFD code, version 2312 [21], specifically with the solver *twoLiquidMixingFoam*. The *twoLiquidMixingFoam* solver in OpenFOAM is specifically designed for simulating the mixing of two incompressible, isothermal fluids. It solves the Navier-Stokes equations for fluid flow along with a transport equation for the phase fraction of one of the fluids. This solver can be adapted for various mixing and diffusion scenarios, making it a suitable choice for your study on the distribution of nitrogen and oxygen in controlled atmosphere treatments.

Although the solver has been validated in numerous scientific studies in the literature, such as those by Abe and Okagaki [22] and Maru et al. [23], a new validation is presented for a case that closely matches the parameters of the present study. Specifically, the mixing process of two miscible fluids in a lid-driven cavity in the laminar regime by Huang et al. [24], where the authors provide experimental data and simulated results. In Figure 2, the comparison of the experimental and simulated horizontal concentration profiles of the heavier fluid is presented, the results of the twoLiquidMixingFoam are presented when the dimensionless time instant is equal to three. It is evident that the twoLiquidMixingFoam results are in close agreement with the experimental data and almost identical to the simulation model provided by Huang et al. [24].

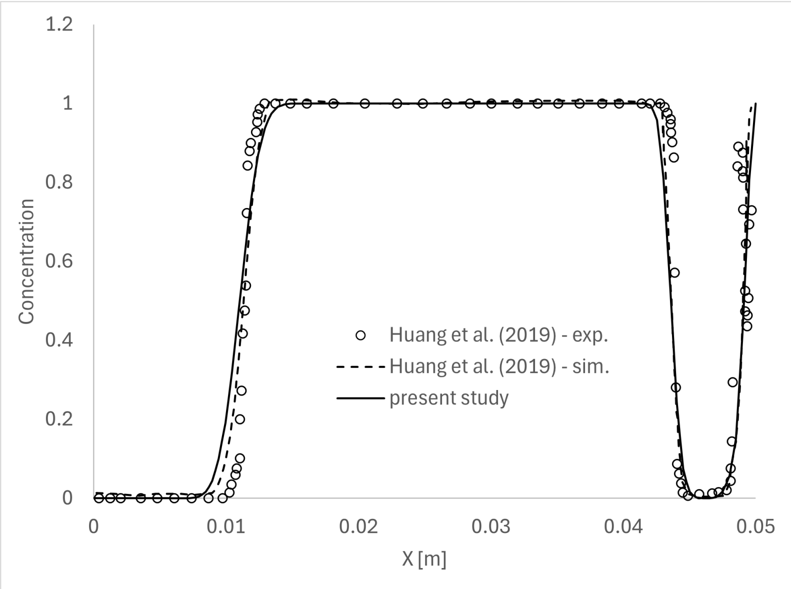

Figure 2. Comparison of the twoLiquidMixingFoam results with the experimental data and simulated results from Huang et al. [24]. Specifically, the horizontal concentration profiles of the heavier fluid when the dimensionless time instant is equal to three.

The governing equations for continuity, momentum and transport for concentration for laminar flow (Reynolds number is equal to $Re = 605$) are:

$$\nabla \cdot \mathbf{U} = 0 \tag{1}$$

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot (\mathbf{U}\mathbf{U}) = -\nabla p + \nabla \cdot (\nu \nabla \mathbf{U}) + \mathbf{g} \tag{2}$$

$$\frac{\partial \alpha_{O_2}}{\partial t} + \nabla \cdot (\mathbf{U}\alpha_{O_2}) = \nabla \cdot (D \nabla \alpha_{O_2}) \tag{3}$$

where t denotes the temporal parameter in seconds [s], x is the spatial parameter measured in meters [m], $\mathbf{U}$ is the velocity field [m/s], ν is the kinematic viscosity, $\mathbf{g}$ is the gravitational acceleration vector, α_{O_2} is the phase fraction of oxygen (the phase fraction of Nitrogen, α_{N_2}, is given by $1 - \alpha_{O_2}$), $p - \rho g h$ is the Hydrostatic Perturbation Pressure [Pa], represents the pressure without the hydrostatic component (minus gravitational potential), D is the binary diffusion coefficient [m^2/s] which for the present study was calculated from Bird et al. [25] equal to 1.944×10^{-5} [m^2/s].

Given the geometry and nature of the problem, a two-dimensional slice was used to reduce computational effort without compromising result accuracy. For this study, a structured orthogonal mesh was employed, with all cells designed as hexahedra to ensure precise modelling. Additionally, the mesh resolution was refined near the walls, inlet, and outlet to accurately capture large gradients. To ensure the accuracy and reliability of the computational fluid dynamics (CFD) simulation, a grid independence study was conducted. This study involved evaluating the time required for the gas concentration in a chamber to reach 1.5% for both its average ($O_{2,avg}$) and minimum ($O_{2,min}$) values across three different grids: Grid G1, Grid G2, and Grid G3, containing 100,000, 160,000, and 220,000 cells, respectively. The results showed that the time for the $O_{2,avg}$ to reach 1.5% was 10.47 h for Grid A, 10.42 h for Grid B, and 10.42 h for Grid C. The differences in these values, when compared to Grid B, were 0.53% for Grid A and 0.05% for Grid C. For the $O_{2,min}$, the times were 11.67 h for Grid A, 11.93 h for Grid B, and 11.76 h for Grid C, with differences of 2.17% for Grid A and 1.42% for Grid C relative to Grid B. These minimal variations indicate that the simulation results are largely independent of the grid size, confirming the grid independence of the CFD simulation. Based on this analysis, Grid B was selected for the remainder of the study to balance computational efficiency and accuracy. Specifically, the grid has a maximum aspect ratio of 7.6. Since the mesh is orthogonal, the mesh non-orthogonality is zero, which is the ideal condition.

In the simulation of fluid flow and species transport using OpenFOAM, various boundary conditions are employed to define how the flow and species concentration behave at the boundaries of the computational domain. These boundary conditions specify the values or behavior of velocity, pressure, and species concentration at different locations such as inlets, outlets, walls, and symmetry planes. For example, at the inlet boundary, the velocity and species concentrations are prescribed based on the known conditions of the incoming flow. At the outlet boundary, conditions were set to allow free outflow, while at walls, no-slip conditions were applied to mimic the physical behaviour of fluids near solid surfaces. Additionally, zero-gradient conditions were used for pressure and species concentration at outlet and walls to represent the absence of flow or diffusion across these boundaries. To ensure stability and convergence of the simulations, OpenFOAM's twoLiquidMixingFoam allows adjustment of the upper limit on the Courant number and the Maximum Interface Courant Number. The Courant number helps maintain numerical stability, as high values can lead to instability and divergence in the solution. The Maximum Interface Courant Number, similar to the Courant number but specific to the phase interface in multiphase flow simulations, ensures accurate and stable resolution of the interface movement between the two liquids. For stability, both parameters should be set below 1. In this study, they were set to 0.5.

3. Results

The CFD simulations provide two-dimensional profiles of oxygen concentration for all cases, as will be shown later. From these profiles, we can extract the time evolution of the maximum oxygen concentration $O_{2,max}$ in the chamber as well as the average oxygen concentration $O_{2,avg}$. In pest control processes using modified atmospheres, the $O_{2,max}$ concentration holds particular importance as practitioners' protocols often refer to this parameter. However, the average concentration also offers valuable insights into the overall status of the chamber and the level of mixing that occurs (small differences between maximum and average values indicate higher mixing of the inserted nitrogen gas and the air).

Figure 3 illustrates these two parameters ($O_{2,max}$ and $O_{2,avg}$). Regarding $O_{2,max}$ (Figure 3A), Case C appears to be the least effective as it fails to reduce the oxygen concentration to the desired levels (1.5%). Cases A and B exhibit similar trends, where $O_{2,max}$ begins to decrease before the first hour of treatment and asymptotically approaches 1%, which matches the output of the nitrogen generator. The target concentration of 1.5% oxygen is achieved after 11.9 and 8.5 h for cases A and B, respectively (see Table 2). Case D emerges as the most effective configuration, achieving the target oxygen concentration of 1.5% after 4.4 h, indicative of a process closer to fully stratified behavior. When a gas enters a chamber in a fully stratified process, it exhibits plug flow behavior, meaning that the gas moves through the chamber without significant mixing or diffusion across its cross-section. In this scenario, the gas maintains distinct layers or strata, with each layer traveling through the chamber at the same velocity and without substantial interaction with adjacent layers. As a result, the concentration profile of the gas remains relatively uniform within each layer, with sharp transitions between adjacent layers. This plug flow behavior is often characterized by a well-defined front or interface between the incoming gas and the gas already present in the chamber, which moves steadily through the chamber without spreading laterally or mixing with the surrounding gas [26,27].

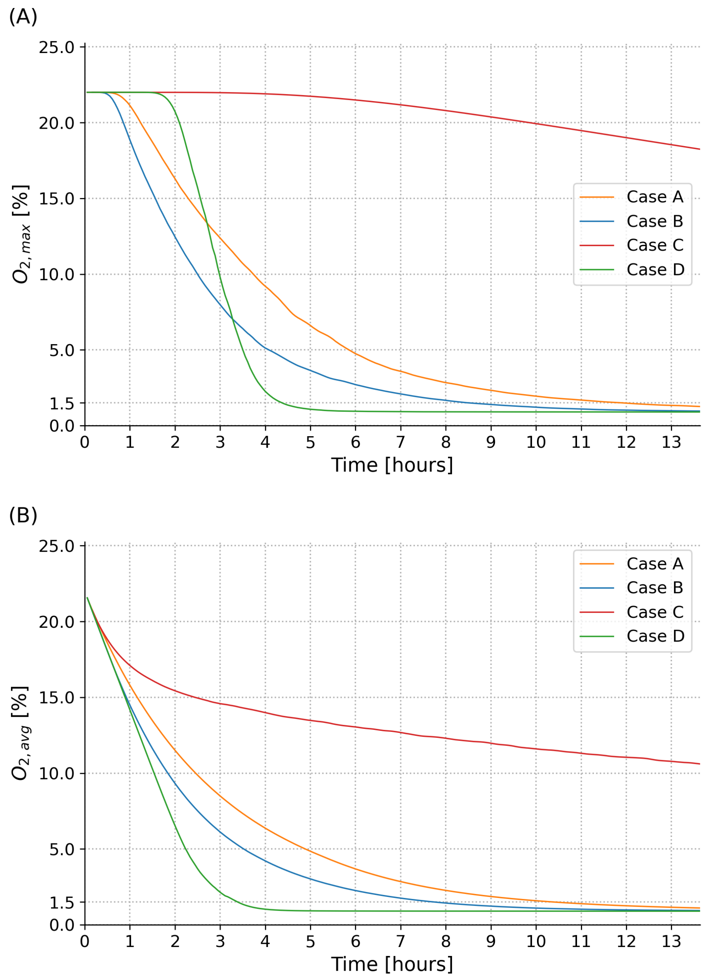

Figure 3. Time evolution of $O_{2,max}$ (**A**) and $O_{2,avg}$ (**B**) concentration for all cases.

To assess the effectiveness of each scenario, we can compare it with the fill time, which represents the duration required for the entire initial gas volume to be replaced by nitrogen from the generator, assuming a plug flow scenario. As mentioned in the preceding section, the fill time is 2.7 h. Table 2 presents these values, which are 4.4, 3.1, and 1.6 for cases A, B, and D, respectively. Case D stands out as the most efficient configuration, with a value of 1.6, indicating that it takes 1.6 times the fill time to reach the desired state. This value is close to the ideal value of 1 and is half the value of Case B (3.1) and even lower than that of Case A. These results suggest that this configuration should be considered as the optimal choice in case other parameters of the process change (e.g., nitrogen flow rate from the generator, chamber dimensions), or at the very least, it should be the initial configuration tested for efficiency. Regarding Case C, the respective value could not be calculated within the simulation time frame, as it would require a significantly longer period to reach completion. Figure 3 shows that even after 13 h, this configuration is still far from reaching the desired concentration, clearly indicating its unfavourable nature.

In terms of $O_{2,avg}$, as shown in Figure 3B, cases A and B show a similar pattern in their respective $O_{2,avg}$ evolution, exhibiting also smaller differences from $O_{2,max}$ as well. This observation suggests a higher degree of mixing (lower stratification), indicating that at any given moment, there are minimal variations in O_2 concentration inside the chamber.

Conversely, the most significant disparities between $O_{2,avg}$ and $O_{2,max}$ are observed in Cases C and D, where the largest differences in O_2 concentration are expected at different locations within the chamber.

Table 2. Time needed for $O_{2,max}$ and $O_{2,avg}$ concentration to reach 1.5% for each case. "N/A" corresponds to very long times that were no simulated.

Case	Time [h] $O_{2,max}$	Time [h] $O_{2,max}/t_{filll}$
A	11.9	4.4
B	8.5	3.1
C	N/A	N/A
D	4.4	1.6

To gain a deeper understanding of why Case D was the most efficient, we look at Figure 4, which gives an insight into the spatial distribution of oxygen within the chamber at 2.7 h (fill time). In Case A, where nitrogen is introduced from the bottom and expelled from the top, there is a small gradient in oxygen concentration. Even though nitrogen is introduced near the bottom and oxygen levels should be higher in the lower levels, the buoyancy forces (nitrogen is less dense than air) cause the nitrogen to move upwards, resulting in higher oxygen levels near the bottom and lower at the top. This indicates that while the configuration is somewhat effective in displacing oxygen, diffusion and buoyancy effects do not result in a clear displacement of oxygen. Case B, with both the inlet and outlet positioned at the bottom, demonstrates a mixing distribution of oxygen but nonetheless at lower oxygen levels (as confirmed from Figure 3B). Case C, where both the inlet and outlet are at the top, exhibits the greatest degree of stratification. The oxygen concentration remains higher (red areas) at lower levels of the chamber, indicating poor penetration of nitrogen and ineffective displacement of oxygen. This configuration seems to fail to achieve the required low oxygen levels. The reason is that the low oxygen layers, which are mostly in the top regions of the chamber (due to buoyancy), exit the chamber from the top outlet before they interact with (and reduce) the oxygen levels in the entire chamber. Any reduction of the O_2 concentration occurs primarily to diffusion. Case D, with the inlet at the top and the outlet at the bottom, emerges as the most promising configuration. Figure 4D confirms that this setup achieves the lowest overall oxygen concentrations, demonstrating effective displacement of oxygen throughout the chamber. Although there are slightly higher oxygen levels at the very bottom (red areas), the majority of the chamber benefits from a uniformly low oxygen environment necessary for asphyxiating insects. This configuration maximizes the downward flow of nitrogen, efficiently pushing oxygen out through the bottom outlet.

Another way to evaluate the two-dimensional results is to study the vertical profile of O_2 concentration (averaged in horizontal planes) within the chamber, specifically after 2.7 h (fill time) for all cases (Figure 5). This method facilitates quantifying the degree of mixing, which, as previously shown, is crucial for determining the most and least efficient inlet/outlet configurations.

For cases A and B, Figure 5 demonstrates that the vertical O_2 concentration differences ($O_{2,max} - O_{2,min}$) are the lowest, 5.3% and 2.7% respectively, quantifying the mixing effects discussed earlier. Case C exhibits the largest O_2 concentration difference (20.8%), attributable to the formation of two distinct concentration zones: the top zone, with the lowest oxygen concentration due to nitrogen entering and exiting from the top, and the lower zone, with high oxygen concentration as nitrogen penetration is limited primarily to diffusion. Case D, identified as the most effective configuration, shows a vertical O_2 concentration difference of 12.1%.

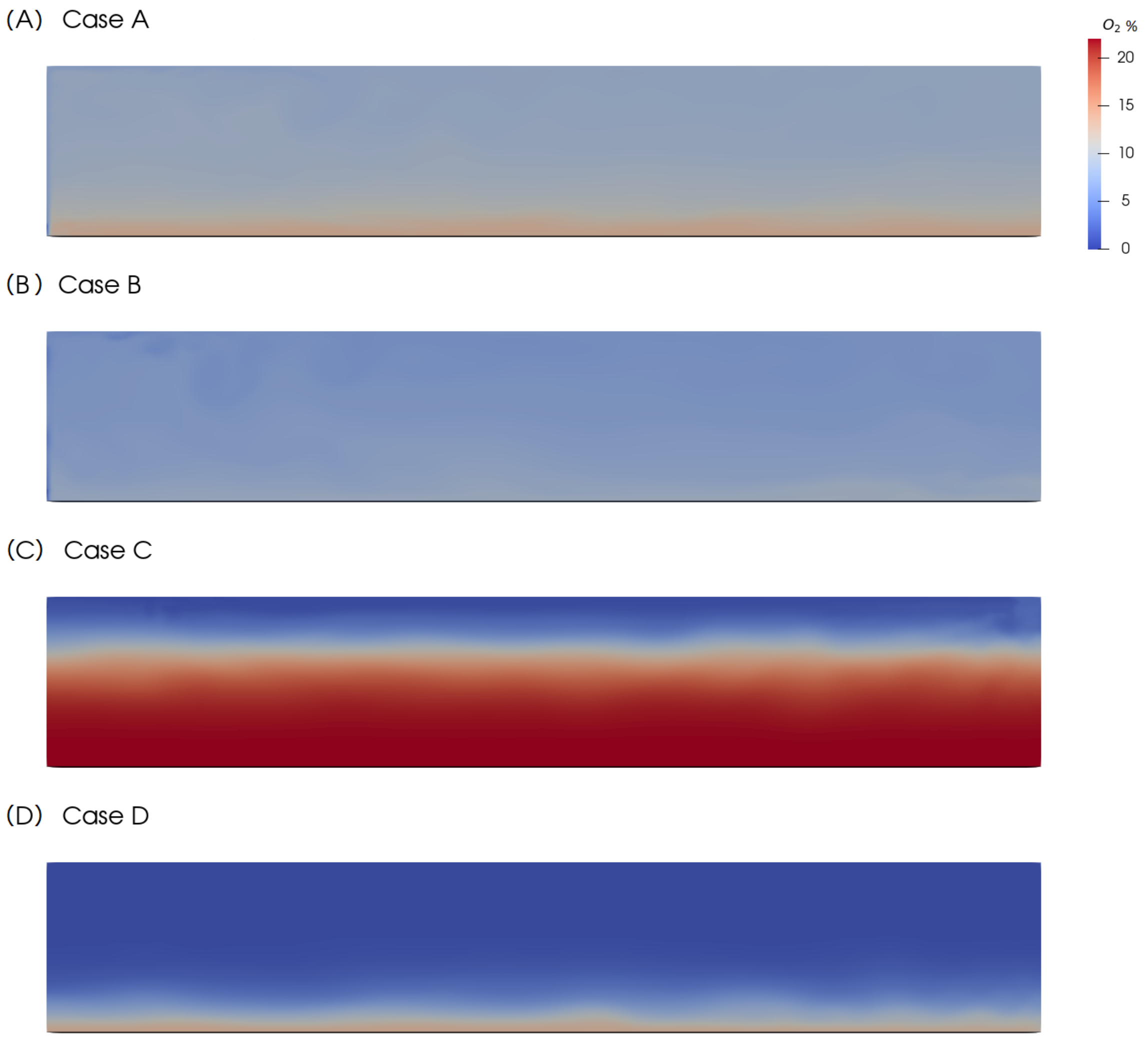

Figure 4. A two -dimensional representation of the O_2 % concentration at time 2.7 h, representing one fill time, for all cases (labelled (**A**–**D**)) tested in this study.

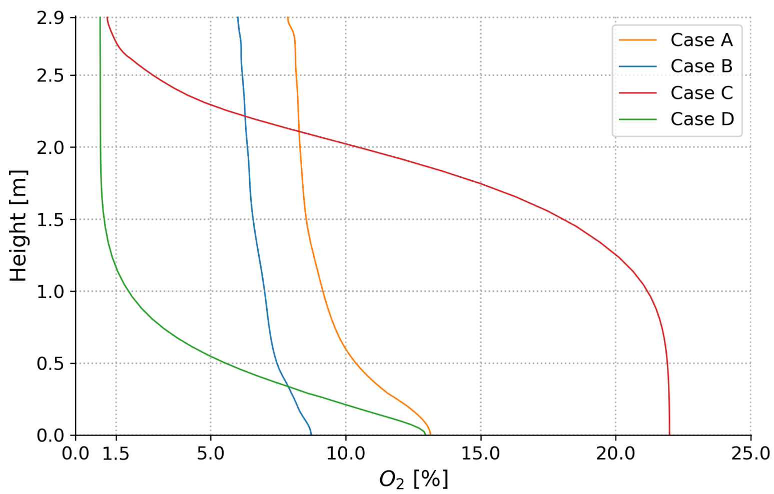

Figure 5. The vertical profile of O_2 concentration (averaged in horizontal planes) within the chamber after 2.7 h (fill time) for all cases.

4. Discussion

Computer simulations have enabled a thorough investigation into the effects of modified atmospheres on insect control. For instance, Kaloudis et al. [14] employed computational simulations using the convection-diffusion equation to study nitrogen penetration and distribution in chamber-contained pallets. They considered two boundary conditions: one where the chamber had already reached a uniform nitrogen concentration of 0.5%, and another where the concentration gradually decreased from atmospheric levels to 0.5%. The present study focuses on identifying the best configuration for the second boundary condition, which Kaloudis et al. [14] noted took approximately six days to reach the desired levels. These lengthy times are subject to optimization, and the present study proposes a mechanism for achieving this.

Considering exposure time, Sakka et al. [20] studied adult populations of both phosphine-resistant and susceptible populations of the red flour beetle, *Tribolium castaneum* (Herbst) (Coleoptera: Tenebrionidae), *O. surinamensis*, and *S. oryzae*. They conducted experiments in commercial nitrogen chambers, exposing the insects to 1% oxygen for varying durations, including 2.5, 3, and 9 days. Similarly, Agrafioti et al. [12] investigated the effects of exposure time and temperature on *O. surinamensis* and *R. dominica*, achieving 100% mortality over exposure times from 2.5 to 9 days and temperatures from 28 to 40 °C. Both studies focused on relatively short exposure times, such as 2.5 days, emphasizing the significance of the present study. In a real-life scenario, the process duration would equal the time needed to reach the desired oxygen levels plus the protocol duration (e.g., 2.5 days). For Case D (which proved to be the optimal inlet/outlet configuration), the entire process would last 64.4 h, whereas for Cases A and B, it would be 71.9 and 68.5 h, respectively. This translates to only a 7.3% delay for Case D, compared to 19.8% and 14.2% delay for Cases A and B, respectively. The delay for Case C would be even higher.

Other examples of successful use of computational methods to optimize pest management include phosphine fumigation. Specifically, Agrafioti et al. [19] modelled the distribution of phosphine gas in six metal silos containing wheat and compared the results with available data from phosphine sensors. During fumigation, a recirculation system was employed to enhance phosphine diffusion. They tested three different scenarios for the recirculation system: (a) Scenario 1, where the recirculation system was used for only 24 h at the beginning of the fumigation; (b) Scenario 2, where the system was used for four consecutive days from the start; and (c) Scenario 3, where the recirculation system was used for approximately 50 h from the beginning. They found that Scenario 3 was the most effective, showing the most uniform distribution in the treated silo compared to the other two scenarios. These results indicate that CFD can establish a methodology for precision fumigation, paralleling the present study's focus on optimizing controlled atmospheres, another major pest control method.

The widespread adoption of modified atmospheres is largely influenced by cost considerations, primarily due to the need for specialized equipment that is often unavailable in conventional fumigation practices. Generally, the use of nitrogen is more expensive than the dominant chemical control methods [3,28]. However, in the long term, investing in nitrogen-based solutions for storage and processing facilities may be justified by the benefits, particularly the environmental advantages of this approach. This study will help to improve the efficiency of the process, thereby reducing operating costs and facilitating the adoption of this environmentally friendly method.

As discussed in the introduction, computational modelling of modified atmospheres remains a relatively under explored research area, and this study contributes towards addressing this gap. However, the complexity and breadth of the subject impose certain limitations, making it impractical to cover all possible scenarios comprehensively within a single investigation. Future research should consider additional factors that could affect gas distribution, such as variations in temperature, humidity, and pressure. Examining these variables would enhance our understanding of the dynamics in modified atmospheres. Moreover, expanding the scope to include different boundary conditions, a variety of agricultural products, and diverse storage structures (e.g., silos) would provide a more robust validation of the simulation model. Integrating insect mortality models into future studies could yield valuable insights, particularly by highlighting specific areas of interest, like the core of the grain bulk. This inclusion would foster a more holistic understanding of the interplay between oxygen distribution and insect control.

5. Conclusions

This study provides insight into the optimal configurations for modified atmosphere treatments in pest control. Using computational fluid dynamics (CFD) simulations, the research identified the most effective inlet and outlet configurations to more quickly achieve the low oxygen levels required to asphyxiate insects. Of the configurations tested, Case D, with the inlet at the top and the outlet at the bottom, proved to be the most efficient. This configuration achieved the target oxygen concentration of 1.5% in the shortest time (4.4 h), demonstrating effective displacement of oxygen throughout the chamber and maximising downward flow of nitrogen. The study highlighted the importance of CFD in understanding these results by providing detailed two dimensional oxygen concentration profiles and vertical oxygen concentration profiles. Although nitrogen-based solutions are generally more expensive than traditional chemical methods, the improved efficiency of the process demonstrated in this study may facilitate wider adoption of this environmentally friendly method. Future research should consider additional factors not covered in this study, such as variations in temperature, humidity and pressure, as well as different boundary conditions, agricultural products and storage structures. The integration of insect mortality models would further improve understanding, particularly in areas such as the core of the grain bulk, thereby promoting a more holistic understanding of oxygen distribution and insect control dynamics.

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