MODELLING AND SIMULATION OF THE STERILIZATION PROCESS OF POUCH PACKAGING IN AN ASEPTIC LINE

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ABSTRACT
Computational Fluid Dynamic (CFD) models were used in this paper to analyze and improve the sterilization process of spouted pouch with a mixture of air and Vaporized Hydrogen Peroxide (VHP) for an aseptic line. In the first part of the work the process of sterilization of spouted pouches has been analyzed using a mixture composed by vaporized hydrogen peroxide and hot sterile air. Simulations allowed reaching the best combination between nozzle position and geometrical shape of output section. In the second part of the work was carried out the simulation of the flow of sterile air in order to obtain the value of flow rate which could ensure the complete removal of the sterilizer with the lowest air consumption. The results obtained ensure a significant reduction of sterile air consumption. Results of simulations have been validated with empirical tests.

Keywords: Aseptic filling, Packaging sterilization, CFD, Design optimization

1. INTRODUCTION

Sterilization of food packaging is one of the most critical phases of aseptic processing (Ferretti et al., 2006; Robertson, 2006). During last ten years many experiments and studies have been performed in order to identify the better sterilizing agent for each combination of product/packaging (Robertson, 2006). Chemicals and physical methods (pulsed light, β and γ radiation) have been mainly investigated as sterilization principle (Farkas, 1999; Riganakosa et al., 1999).

Regarding chemical methods, the main problem is due to the temperature of the chemical agent allowable during the packaging treatment. Hydrogen Peroxide reaches a good efficacy only having temperature higher than 70°C, so if the packaging material to treat has a lower point of glass transition (i.e for PET 69°C), it is not possible to use liquid solution, at the risk of damage the packaging. For this reason an addition of peroxiacetic acid in percentage of about 1% has been frequently used, in order to decrease the temperature of action of the hydrogen peroxide solution. However this addition increase the cost of the solution, so many company tried to use only Hydrogen peroxide in vapor condition (Yun an Sastry, 2007).

The two techniques manly adopted in the last ten years was Vaporized Hydrogen Peroxide (VHP) and Condensing Hydrogen Peroxide (CHP). The first method does not produce vapor condensation on the inner side of the packaging, instead CHP method want create this condensation in order to be more powerful on microbial reduction. These methods has been tested by several authors for many food packaging in order to optimize the sterilization process (Klapes and Vesley, 1990).

Sterilization of flexible containers shows, however, additional problems during the removal of the sterilizer agent, which is complicated by the small size of the exit hole and by the type of material (Castle et al, 1995; Abdul Ghani, 2001). For this reason it was decided to analyze and simulate both the VHP sterilization process and the removal of sterilizing agent of pouch packaging. The work is therefore divided into two parts.

In the first part of the work the process of sterilization of spouted pouches has been analyzed using a mixture composed of VHP and hot sterile air, while the aim of the second part has been the evaluation and optimization of the removal process of the sterilizing mixture using sterile air. This last phase is used to obtain a low residual value of hydrogen peroxide inside the packages compatible with the values imposed by regulations. Especially, the maximum residual value of hydrogen peroxide fixed by FDA is 0.5 ppm.

Concerning the sterilization process the first goal was to determine the optimal relative position between the sterilization nozzle and the envelope, ensuring an

adequate speed of the flow in each zone of the inner pouch volume. The second aim was to optimize the flow of VHP by varying the nozzle shape.

The objective of the removal process of the sterilizing solution was to evaluate the best configuration of the nozzle, relative position and configuration, and the flow rate value that minimizes the amount of sterile air necessary to remove the residual hydrogen peroxide.

2. MATERIALS & METHODS

The process analysed is the sterilization of the packaging pouch in a pilot plant simulating the working of an aseptic line.

The system analyzed is composed of a sterilization station with a single nozzle spraying the sterilizing solution inside the pouch, and of a removal station of this sterilizing agent. In both of these stations, the nozzles have an overall height of 200 mm and an outlet section with a diameter of 2.5 mm. This form can be modified as required. The pouch pack has a very complex geometry, with a total height of 170 mm, a maximum width of 90 mm, a maximum depth of 53 mm and an overall volume of 340 cm3.

The sterilization is obtained from a mixture of air and hydrogen peroxide. The hydrogen peroxide at 30% of concentration is vaporized in a plate maintained at 200°C. This solution is subsequently mixed with a flow of sterile hot air that has a rate of 2000 Nl/h. The concentration of hydrogen peroxide which should arrive in each envelope is 4000 ppm. The temperature of the whole system is maintained at 55°C to avoid the problem of condensation. The condensation of sterilizing mixture would make it impossible to remove and obtain a residual value in compliance with the regulations.

After the sterilization phase of the pouch, the sterilizer is removed through a flow of sterile air. The removal of hydrogen peroxide is carried out with a nozzle equal to that used in the sterilization phase. The temperature of the air is about 60°C and the process starts 15second after the end of the previous phase. The injection of hot air has to be continued until the amount of Hydrogen peroxide inside the filled pouch decrease under 0,5ppm.

The simulation process has been carried out by means of a CFD commercial code, "Flow Simulation© (Dassault Systèmes SolidWorks Corporation). 3D CAD model of both the nozzle and the pouch have been created by SolidWorks© software.

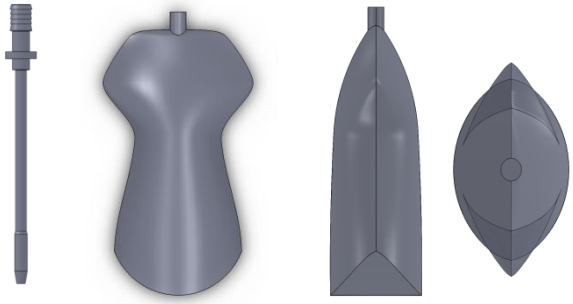


Figure 1: 3D CAD models of nozzle and pouch

The fluid adopted for the simulation was only air because Flow Simulation can't simulate a fluid composed by a mixture of air and hydrogen peroxide. However, this approximation does not create significant problems, being the volume of air approximately 99% of the composition of the mixture.

The turbulence model adopted was the Standard k-ε. The k-ε turbulence models is one of the most used in order to analyse this kind of problems (Ferziger and Peric, 2002; Margaris and Ghiaus, 2006; Bottani et al, 2008). It is part of the Reynolds Averaged Navier-Stokes models (RANS), which consider the average time of the speed to which add terms of fluctuation. In particular, the k-ε is a model with two equations, which means that it includes two additional equations to the classical ones to represent the properties of the turbulent flow.

In this model, the turbulent viscosity μ_t is computed according to the following equation:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

where ρ is the density while turbulent kinetic energy k and its dissipation rate ε are derived from the resolution of the following set of equations:

$$\frac{\partial}{\partial x_j}(\rho u_j k) = \frac{\partial}{\partial x_j}\left[\frac{\mu_{eff}}{\sigma_k}\frac{\partial k}{\partial x_j}\right] + \mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial u_i}{\partial x_j} - \rho\varepsilon$$

$$\frac{\partial}{\partial x_j}(\rho u_j k) = \frac{\partial}{\partial x_j}\left[\frac{\mu_{eff}}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right] + C_{\varepsilon 1}\frac{\varepsilon}{k}\mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial u_i}{\partial x_j} - \rho C_{\varepsilon 2}\frac{\varepsilon^2}{k}$$

$$\mu_{eff} = \mu + \mu_t$$

being μ the molecular viscosity, μ_t the turbulent viscosity of the fluid.

2.1. Mesh setting for the volume of the fluid

The whole body of the pouch is divided into a finite number of volumes on which the analysis is carried out. In "Flow Simulation©" these volumes are cube-shaped.

The number of cells used in the simulations was determined starting from a coarse meshing gradually refined, evaluating the changes in the results. The final mesh was determined when increasing the fineness of the mesh there were not significant improvements in the results.

The mesh was realized initially by creating a uniform subdivision, with a subsequent thickening in the critical areas of the fluid volume. In particular, finer mesh was used near the outlet section of the nozzle,

where is foreseeable that the shear rates would be higher, and close to the wall of the pouch, in order to simulate accurately the flow boundary layer. Since the pouch has a double symmetry, the simulations were carried out in a quarter of volume. This allowed us to optimize simulations run time using mesh with a high level of refinement.

The final mesh consists of about 150.000 cells in the first processing. In the process of sterilizing removal the number of cells has been reduced because the analysis is time-dependent and requires more computational resources.

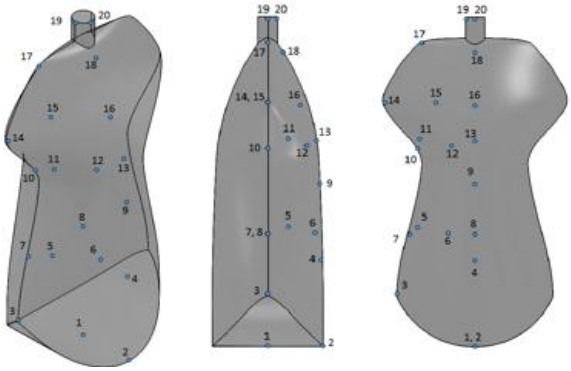


Figure 2: mesh adopted in simulation

With the aim of identifying the values of the flow parameters in significant points of the volume, 20 representative points have been selected, in critical positions, for the sterilization process. Each simulation permits the evaluation of the parameter values in each point.

2.2. Simulation settings

The simulations carried out for the sterilization process were stationary. It is not necessary to show the behaviour during the initial phase, but represent the process at the end of transitory time when the dynamics of the flow becomes stationary. Not considering the initial transitory time does not cause an excessive loss of information.

Two series of simulations were carried out. In the first series eight simulations has been designed with the aim to obtaining a better position of the nozzle. The second series consist of six simulations performed to get an optimized form of the nozzle.

The second series of the simulations concerns the optimization of the sterilizing agent removal. The objective of this phase is to assess the time required by the hot air to remove the sterilizing agent, composed by air and hydrogen peroxide.

Time-dependent simulations have been realized to evaluate the time needed to remove the sterilizing solution and replace it with sterile air. These simulations show the dynamic of the evacuation with a time step of 0.1 seconds. At the beginning the whole volume was full of the mixture. The removal of the hydrogen peroxide starts when the nozzle, with the same shape of the one used in the first simulations, begins to blow sterile air inside the pouch. The flow of sterile air taken in the first round of simulations is 2000 Nl/h. In order to carry out the simulations it was necessary to adopt a simplification. Since the code "Flow Simulation©" is not able to simulate a mixture of air-hydrogen peroxide, only air at 2 different temperatures was used, in order to distinguish the two fluids (mixture sterilizing and sterile air). Secondly the coefficient of thermal conductivity of the air has been reduced to avoid having results skewed by the phenomenon of heat transfer.

Two series of simulations have been designed. The first series consists of six simulations to obtain a better position and shape of the nozzle. In the second series seven simulations have been performed, with different flow rate of sterile air to find out which flow rate permits to reduce the amount of sterile air consumed.

In this case it was necessary to decrease the mesh refinement level in order to reducing the run time simulation without compromising the results reliability

3. RESULTS

3.1. Optimization of sterilization process

In the first phase eight simulations were carried out with different nozzle positions.

The first simulation was performed with the nozzle at a distance of 15 mm from the bottom of the pack . The next simulations were performed with step of 15 mm.

Table 1: simulations realized with different nozzle position

Simulation Number	Distance nozzle – bottom pouch (mm)	Simulation Number	Distance nozzle – bottom pouch (mm)
1	15	5	75
2	30	6	90
3	45	7	105
4	60	8	120

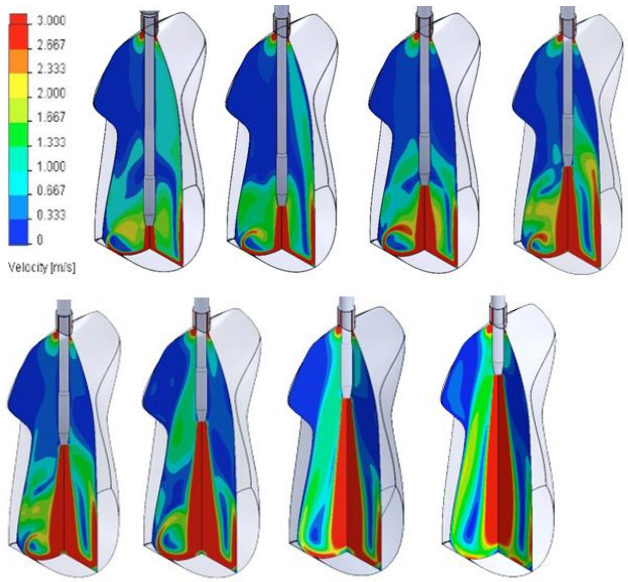
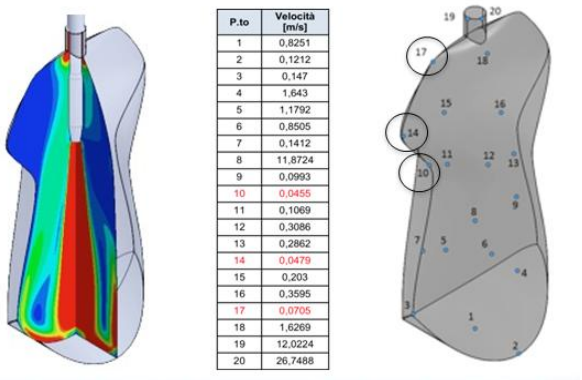


Figure 3: Velocity of the sterilizer

As clearly marked in Figure 3, the conclusions that can be assumed from this first phase of simulations are the following:

- In the first simulations, where the nozzle is in a lower position in the box, the flow of the sterilizing agent reaches a high rate near the bottom of the pouch . In the upper part instead there are large areas at very low speed. The tests performed with the nozzle in upper positions have however good velocity in the lower part and a more uniform flow at the top. The simulations 6, 7 and 8 are those that distribute more evenly the speeds.
- In all simulations carried out, the lateral areas of the upper part of the pouch never reaches significant rate.

For the reasons just mentioned the best position to put the nozzle during the sterilization phase appears to be closer to position 7, in which the nozzle has a distance of 105 mm from the bottom of the envelope. The problem to be solved is related to the low speed in the zones of the upper side. This problem can be solved by changing the nozzle shape. Figure 4 shows simulation 7: as can be seen from the related chart the speed of the fluid in the circled points is very low.



P.to	Velocità [m/s]
1	0,8251
2	0,1212
3	0,147
4	1,643
5	1,1792
6	0,8505
7	0,1412
8	11,8724
9	0,0993
10	0,0455
11	0,1069
12	0,3086
13	0,2862
14	0,0479
15	0,203
16	0,3595
17	0,0705
18	1,6269
19	12,0224
20	26,7488

Figure 4: Air velocity: simulation 7

The problem of low velocity of the mixture in the lateral zones of the upper side of the pouch could be solved by introducing holes on the surface of the nozzle. Some simulations have been made introducing 4 holes of a radius of 2mm, which have been placed at a distance of 15 mm from the exit section of the nozzle.

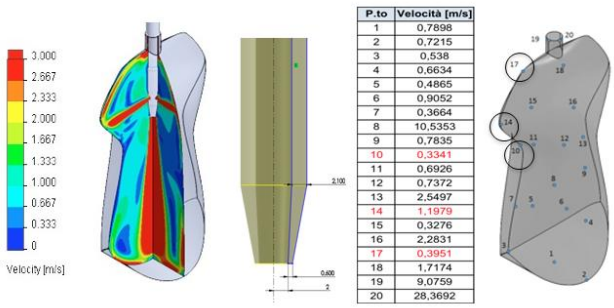
Two parameters, that could be potentially critical in determining the velocity profile of the mixture, are the radius of the outlet section and the thickness of the nozzle closeto the holes. Six simulations has been realized, all with the same position of the nozzle as in simulation 7, varying the two parameters.

Table 2: simulations with different nozzle geometry

Number of simulation	Radius of the outlet section (mm)	Thickness of the nozzle in correspondence to holes (mm)
1	2,5	2,1
2	2,25	2,1
3	2	2,1
4	2,5	1
5	2,25	1
6	2	1

Figure 5: Nozzle modified by the insertion of 4 holes

Simulation 3 shows the best solution found. The nozzle has the outlet section with a radius of 2 mm and a thickness close to the holes of 2.1 mm. The reduction of thickness near to the holes, did not produced improvements because the speed did not achieve significant values particularly in the frontal area of the central part of the pouch.



P.to	Velocità [m/s]
1	0,7898
2	0,7215
3	0,538
4	0,6634
5	0,4865
6	0,9052
7	0,3664
8	10,5353
9	0,7835
10	0,3341
11	0,6926
12	0,7372
13	2,5497
14	1,1979
15	0,3276
16	2,2831
17	0,3951
18	1,7174
19	9,0759
20	28,3692

Figure 6: map of speeds and local values of speed of simulation 3, which has guaranteed the most uniform flow

3.2. Removal process of the sterilizer

Six simulations has been performed in the first phase as summarized in Table 3. In these simulations the flow rate of sterile air is set at 2000 Nl/h.

Table 3: simulations with each nozzle position and geometry

Number of simulation	Nozzle position	Nozzle typology
1	high	nozzle without lateral holes
2	Middle	nozzle without lateral holes
3	Low	nozzle without lateral holes
4	high	nozze with 4 lateral holes with radius of 2 mm
5	Middle	nozze with 4 lateral holes with radius of 2 mm
6	Low	nozze with 4 lateral holes with radius of 2 mm

Simulations were also carried out with a change in the exit section and the thickness of the nozzle, as in the

previous simulation series. The results were very similar to simulations 4, 5 and 6, with a slight worsening in terms of removal time. The upper position has a distance between the nozzle and the bottom of the envelope of 110 mm, the middle position of 70 mm and the lower position 30 mm.

The best solution is that of simulation 5 in which the removal of the sterilizing agent is achieved in 4,6 seconds.

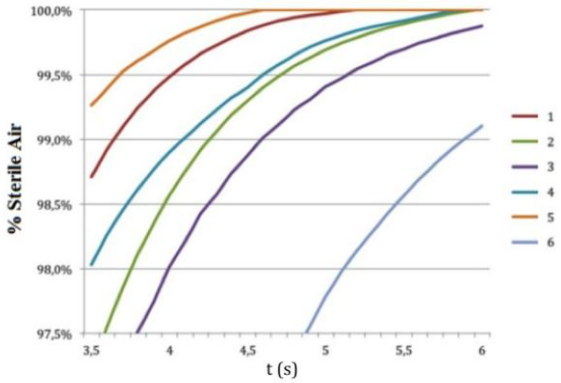


Figure 7: Comparison of percentages' trends of sterile air in the 10 most critical points for the different simulations

Figure 8 shows the trend in the removal process over the time that picks out the replacement of the sterilizer with sterile air. The colour blue corresponds to the sterilizer and the red to the sterile air. As previously explained the simulated process is not the same process of removing the sterilizer with sterile air, because it is not permitted by the software. We have simulated the two fluids with air, and to distinguish the two fluids we have assigned them different temperatures. The VHP assumed a temperature of 55°C and the sterile air at temperature of 200°C. Values of kinematic viscosity and density were set not dependent on the temperature and equal to air values at 55°C Depending on the temperature detected in any point is possible to go back to what percentage of the two fluids is present in that instant. In the coloured map is assigned the blue colour to the areas with a temperature below 198°C and the red colour for temperature between 198°C and 200°C.

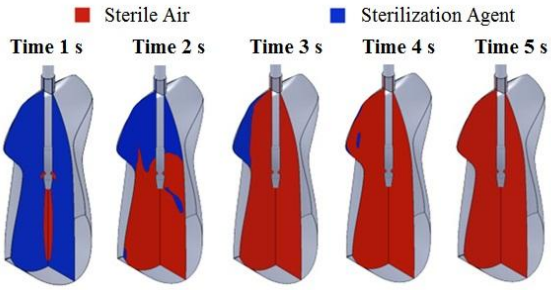


Figure 8: dynamics of the removal process of he sterilizer in the configuration of simulation 5

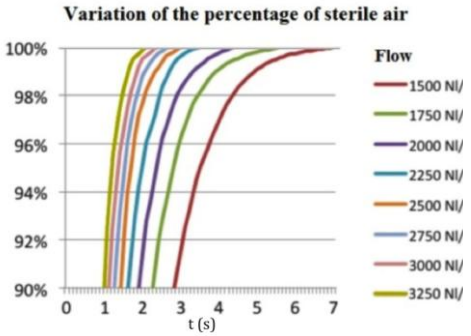
In the simulations just explained the air flow rate was set at 2000 Nl/h as in all the tests.

The objective of this second phase is to determine the optimal flow of sterile air. The optimal range is the one that can get the best compromise between the amount of air used and the size and complexity of the removal station. The objective is therefore to have a flow that minimizes the amount of air needed and a low rinsing time in order to reach a high rate and consequently a reduced number of nozzles. To do this, 7 additional simulations were carried out with the same shape as in simulation 5,with different flow rate of sterile air. The rate values are those reported in Table 4.

Table 4: set flow rate in the last simulations

Number of simulation	Flow rate (Nl/h)
1	1500
2	1750
3	2250
4	2500
5	2750
6	3000
7	3250

The obtained time values of sterilizer removal are summarized in Figure 9.



Flow rate (Nl/h)	Removal time (s)
1500	7
1750	5,7
2000	4,6
2250	3,5
2500	3
2750	2,7
3000	2,5
3250	2,4

Figure 9: time of sterilizer removal

The needed amount of sterile air is given by the product of flow rate and minimum removal time of the sterilizing agent. The minimum amount of sterile air is achieved with a flow rate of 2750 Nl/h (Figure 10). Values slightly higher are obtained with flow rates of 2500 and 3000 Nl/h. It is possible to conclude that the optimal range of flow rate is between 2500 and 3000 Nl/h.

Flow Rate (Nl/h)	Amount of sterile air (Nl)
1500	2,91
1750	2,77
2000	2,56
2250	2,18
2500	2,08
2750	2,06
3000	2,08
3250	2,17

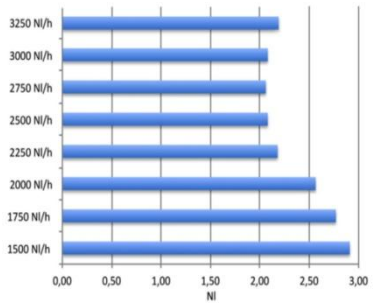


Figure 10: amount of sterile air required for the process

The increase in flow rate, compared to the previous case, permits a reduction of sterile air and allows to reduce the number of nozzles required for this process. The reduction of nozzles can be calculated as follows.

$$\text{Reduction of nozzles [\%]} = \frac{4{,}4\text{-}2{,}7}{4{,}4} \times 100 = 39\%$$

The values of 4.4seconds and 2.7seconds are respectively the removal time in the case of 2000 Nl/h and the removal time in the case of 2750 Nl/h.

The time required to remove the sterilizer has been validated by empirical tests. The test has been realized by executing the normal process of sterilization and then injecting sterile air with the flow rate of 2750 Nl/h. The flushing time of sterile air inside the envelope was:

- 3 seconds in the first test
- 5 seconds in the second test

For each test carried out at the end of this process the bag was filled with 330 ml of water without mineral salts, and shacked to ensure that all the residual hydrogen peroxide could dissolve in the solution. To measure the residual value a tool based on reflectometry technique has been used. After this a reagent strip was put inside the pouch for 15 seconds and subsequently inserted into the detector. The concentration is calculated as a function of the redox reaction that occurs. The strips are able to measure the residual values between 0.2 ppm and 20 ppm. The following table shows the concentration reported in ppm.

Table 5: residual of hydrogen peroxide in the empirical tests

Flow rate	Time	Residual
2750 Nl/h	3 s	0,6 ppm
	5 s	0,2 ppm

The data obtained are coherent to the one calculated, even if they show a longer time. In fact, the number of ppm after 3 seconds is slightly higher than the maximum allowed (0,5 ppm), while in the calculation carried out after 2.7 seconds the condition of sterility would be reached. After 5 seconds the hydrogen peroxide is completely removed (the indicator always measures a minimum of 0.2 ppm).

4. CONCLUSION

The aim of this study was to analyze and improve the sterilization process of spouted pouch for an aseptic line.

The first part of the research was aimed at determining the position and the geometry of the nozzle, which could ensure a flow of sterilizing solution with significant velocity values in each part of the pouch, avoiding areas where the speeds are too low. Simulations allowed reaching the best combination between nozzle position and geometrical shape of output section.

In the second part the removal process of sterilizing agent has been analyzed in order to estimate the time required for this operation. Inside the pouch was introduced hydrogen peroxide at a concentration of 5000 ppm and the maximum residual value that may remain in the finished product is 0.5 ppm. Among the simulations carried out the one that has achieved the best results has the nozzle located 70 mm above the bottom of the envelope, with 4 lateral holes that have the same characteristics of those included in the solution obtained in the previous phase. This solution guarantees the complete removal of the sterilizer in the shortest possible time (4.6 seconds), assuming a flow of sterile air of 2000 Nl/h.

The last phase of this research has tried to optimize the flow of sterile air in order to obtain the value of flow rate which could ensure the complete removal of the sterilizer with the lowest air consumption. The optimal value of flow rate was 2750 Nl/h and the optimal range is between 2500 and 3000 Nl/h. Taking as flow rate 2750 Nl/h a significant savings of required quantity of sterile air has been obtained. In particular, the consumption for each pouch has become 2.08 Nl instead of 2.44 Nl that was the amount of the case previously chosen. As a second important advantage, this choice reduces the number of nozzles and consequently the size and complexity of the carousel.

For the sterilization process it would be important to perform experimental tests to evaluate the effect of the obtained improvement. New experimental tests should be carried out. for the process of sterilizer removal in order to calculate the residual concentration of hydrogen peroxide with more precise equipments that allow to obtain data with a lower margin of error.

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