MODELLING AND MULTI-OBJECTIVE OPTIMIZATION OF THE VHP STERILIZATION PROCESS OF POUCH PACKAGING

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ABSTRACT
Aseptic filling technology of Spouted Pouch packaging, even more used in the beverages sector, requires a very complex sterilization and rinsing of the packaging before filling.

This work aims to optimize the sterilization process of a pouch packaging used in aseptic technology. Starting from a fixed position of the nozzle inside the pouch, this work goals to varying the flow rate through the nozzle and the process time, in order to ensure the contact between H_2O_2 solution and all zone of the packaging wall, so to optimize the sterilization process. The analysed sterilization process adopts a mixture composed by vaporized hydrogen peroxide and hot sterile air.

This problem has been resolved using a multi-objective optimisation with the mains objectives to minimize the consumption of H_2O_2 and the relatives costs and maximize the sterilization efficacy on the packaging volume in a defined time.

Keywords: pouch packaging, VHP sterilization, multi-objective optimization, ModeFrontier.

1. INTRODUCTION

The Sterilization of food packaging is one of the most critical phases of the aseptic processing (Ferretti et al., 2006). During the last ten years many experiments and studies have been performed in order to identify the best sterilizing agent for each combination of product-packaging (Robertson, 2006; Ansari and Datta, 2003). In particular, polymeric-based packaging has assumed a main role in aseptic packaging thanks to its economic convenience, an easy stock and transport. On these kinds of packaging materials, both Chemicals (wet peroxide acetic acid, wet and vaporized hydrogen peroxide, etc..) and physical methods (pulsed light, β and γ radiation) have been adopted as sterilization principle (Abreu and Faria, 2004; Riganakosa et al., 1999; Farkas, 1998).

Regarding chemical methods, the main problem is caused by the temperature of the chemical agent reached during the polymeric packaging treatment. Hydrogen Peroxide reaches a good efficacy only at a 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, with the risk of damaging the packaging. For this reason an addition of peroxide acetic acid at a 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 companies tried to use only Hydrogen peroxide in a vaporized form (Yun and Sastry, 2007).

The two techniques primarily adopting Hydrogen Peroxide in vapour condition were the "Vaporized Hydrogen Peroxide" (VHP) and "Condensed Hydrogen Peroxide" (CHP) (Cerny, 1992). The first method does not produce vapour condensation on the inner side of the packaging, thanks to the use of a pre-heating section; instead CHP method wants produce this condensation in order to be more powerful on microbial reduction, using a packaging not pre-heated. Both these methods have been experimentally tested by several authors for many food packaging in order to optimize the sterilization process (Klapes and Vesley, 1990; Cerny, 1992).

The application of these latter sterilization techniques on flexible containers shows, also, additional problems about the removal process of the sterilizing 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 only VHP method is currently adopted in the food sector, according to its better removal property of hydrogen peroxide from the packaging surface.

In order to simulate the behaviour of this latter technology, numerical simulations could be able to predict the velocity and the concentration of the chemical agent inside the pouch (Patrick Kirchner, 2013). In some cases Computational Fluid Dynamics (CFD) analysis is used to investigate and to optimize industrial beverage processes, i.e. filling, rinsing and empting. Instead, in the case of sterilization using vaporized solutions only one author recently try to approach the problem using CFD methods, mainly due to the complexity of simulate two different vapour component acting simultaneously (Qian Zou, 2006, Shao-Ping Wang et al, ,2004).

Based on these premises, this work aims to optimize the sterilization process of a pouch packaging

used in aseptic technology. Starting from a fixed position of the nozzle inside the pouch, this work goals to simulate the process, varying the flow rate through the nozzle and the process time, in order to ensure the contact between H_2O_2 solution and all zone of the packaging wall, so to optimize the sterilization process.

This work then is divided in two parts: the first one concerns the simulation and modelling the physic condition of the sterilization process on the pouch, and the second one regards the optimization of the process with find the bests configuration.

In the first part of this work, a multicomponent CFD models were used to simulate the Vaporized Hydrogen Peroxide (VHP) sterilization process of spouted pouches. The CFD simulations were in a transient state, being necessary to show the behaviour during the initial phase and because it is important to determinate the correct sterilization time. The use of transient simulations allows testing combinations between variables in order to optimize also the time of treatment. For the first part ANSYS CFX software was used.

In the second part of the work the CFX software was implemented in an optimization tool (ModeFrontier software). Before any optimization, the problem must first be modelled. A multi-objective optimization task considers several conflicting objectives simultaneously. In such a case, there is usually no single optimal solution, but a set of alternatives with different trade-offs, called Pareto optimal solutions, or non-dominated solutions. Despite the existence of multiple Pareto optimal solutions, in practice, usually only one of these solutions is to be chosen. Thus, compared to single-objective optimization problems, in multi-objective optimization, there are at least two equally important tasks: an optimization task for finding Pareto optimal solutions (involving a computer-based procedure) and a decision-making task for choosing a single most preferred solution. All the optimization analysis were performed using Mode Frontier software. In this software we designed a workflow, where is necessary to specify the logic node and the algorithm which will generate all possible allowed combinations. In this case, the logic node was connected to ANSYS CFX.

2. MATERIAL AND METHODS

2.1 Materials

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 2,000 Nl/h. The concentration of hydrogen peroxide which should arrive in each envelope is 5,000 ppm. The temperature of the whole system is maintained at 55°C to avoid the problem of condensation. The condensation of the sterilizing mixture would make it impossible to remove and obtains a residual value in compliance with the regulations. 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 cm^3.

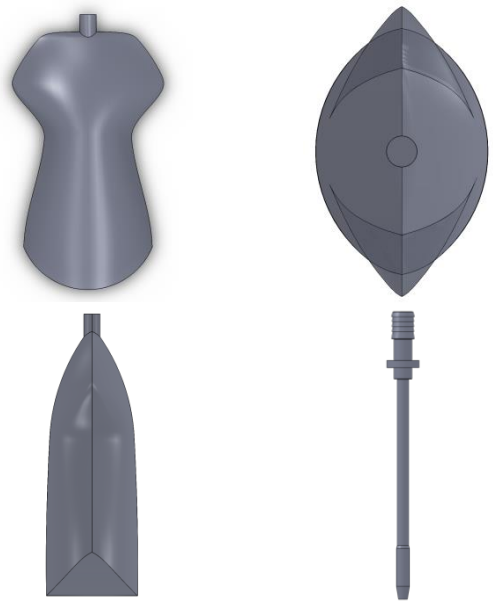


Figure 1. Different view of pouch packaging and sterilization nozzle

2.2 Modelling

2.2.1 CFD Modelling

The CFD simulations have been performed using ANSYS CFX 14.5 version, which allows simulating multi component fluids and to analyse this problem in a more reliable way. One component in each phase must be calculated using a constraint component in the same way as for single-phase multicomponent flow.

For a multicomponent fluid, additional equations must be solved to determine how the components of the fluid are transported within the fluid.

The variation of the properties for a single component influence the global system. Each component has its own equation for conservation of mass. After Reynolds-averaging can be expressed in tensor notation as:

$$\frac{\delta \tilde{\rho}_i}{\delta t} + \frac{\delta (\bar{\rho}_i \bar{U}_j)}{\delta x_j} = -\frac{\delta}{\delta x_j}\left[\rho_i(\tilde{U}_{ij} - \tilde{U}_j) - \overline{\rho_i'' U_f''}\right] + S_i \qquad (1)$$

where:

$\tilde{\rho_i}$ is the mass-average density of fluid component i in the mixture

$\tilde{U}_j = \sum \frac{(\bar{\rho}_i \bar{U}_{ij})}{\bar{\rho}}$ is the mass-average velocity field,

$\tilde{U}_{ij}$ is the mass-average velocity of fluid component i,

$\rho_i(\tilde{U}_{ij} - \tilde{U}_j)$ is the relative mass flux,

S_i is the source term for component i which includes the effects of chemical reactions.

The physical properties of general multicomponent mixtures are treated using the assumption that the components form an ideal mixture, i.e. a mixture of components such that the properties of the mixture can be calculated directly from the properties of the components and their proportions in the mixture.

Thus, the mixture density ρ may be calculated from the mass fractions Yi and the thermodynamic density of each component ρi, which may require knowledge of the mixture temperature and pressure, as well as an appropriate equation of state for each component.

$$\frac{1}{\rho} = \sum_{i=A,B\ldots}^{N_C} \frac{Y_i}{\langle \rho_i \rangle} \quad (2)$$

Extending the Reynolds-averaged conservation equation for energy of a single component fluid for multicomponent fluids involves adding an additional diffusion term. In the special case that all species diffusivities are the same and equal to thermal conductivity divided by specific heat capacity, the energy equation is the following:

$$\frac{\delta}{\delta t}(\rho H) - \frac{\delta P}{\delta t} + \frac{\delta}{\delta x_j}(\rho U_j H) = \frac{\delta}{\delta x_j}\left[\left(\frac{\lambda}{C_p} + \frac{\mu}{Pr_t}\right)\frac{\delta h}{\delta x_j}\right] + S_E \quad (3)$$

This equation has the advantage that only a single diffusion term needs to be assembled, rather than one for each component plus one for heat conduction. This can significantly reduce numerical cost, in particular when the fluid consists of a large number of components. The turbulence model adopted was the Standard k-ε. The k-ε turbulence models is one of the most used to solve 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.

The fluid domain of the pouch was obtained using ICEM CFD, the modeller associated with ANSYS CFX. The volume of the pouch is divided into a finite number of volumes on which the analysis is carried out. Figure 2 shows the generated mesh used for the calculation: an unstructured tetrahedral meshing scheme was used.

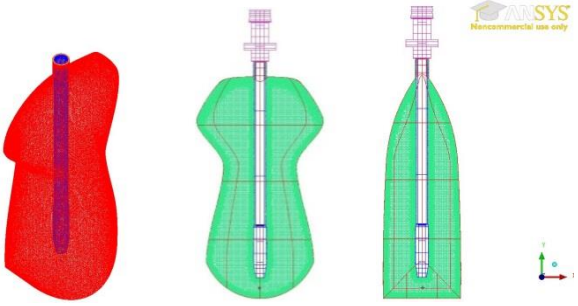


Figure 2. Pouch mesh (for the surface and the volume)

The number of cells used in the simulations was determined starting from a coarse meshing gradually refined, evaluating the changes in the results. In particular, a finer mesh was used near the outlet section of the nozzle, where it 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. The final mesh was determined when increasing the fineness of the mesh there were no significant improvements in the results. The overall number of cells created is about 4,100,000.

2.2.2 Optimisation Modelling

The optimization modelling is the most important part of the process, because it is necessary to specify the optimization strategy that will be used. ModeFrontier software (version 4.4.2) has been adopted for this study.

Optimization process starts with the workflow creation (Figure 3).

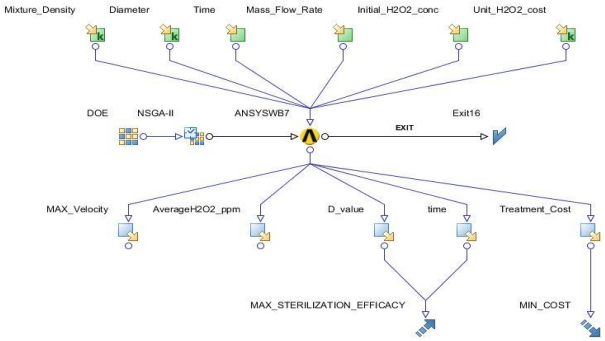


Figure 3. ModeFrontier workflow

The workflow is composed by a process flow and a data flow. The process flow describes the sequences of actions and the data flow describes which data should be moved from one step to another.

First of all, the input variables of the system were defined. In particular, six input were individuated: three of them like a constant and the other three like a variable. In this work, input like the mass flow rate, the initial concentration of H_2O_2 and the time of the sterilization process were kept variable in order to assess the optimal configurations in according to the variation of these particular three inputs.

All the input parameters are defined by dedicated nodes, which specify their range of variation, and they are all linked to the application node. In this work, the Ansys Workbench node was implemented. Table 1 shows the input name and the relative range of values.

Input variables	Type	Range of Values
Mixture density	Constant	1.18 [kg/m^3]
Diameter nozzle	Constant	0.005 [m]
Unit cost H_2O_2	Constant	0.57 [€/kg]
Mass flow rate	Variable	[0.1 l/s; 0.5 l/s]
Initial H_2O_2 conc	Variable	[0.0015; 0.0050]
Time	Variable	[5 s; 10 s]

Table 1. Input variables

Hence the outputs of the system were set. In the model, the outputs have been selected in order to optimize some of them. In particular, the maximum velocity, the final concentration of H_2O_2 expressed in ppm, the treatment cost for each bottle and the treatment efficacy were calculated (Table 2).

Output variables	
Max velocity	Mass flow rate) / (density · surface)
Final average PPM	Ave(H_2O_2.Mass Fraction)·1000000
Treatment cost	Unit Cost · Mass flow rate · Time
Decimal reduction value (D)	4901,5·(AveragePPM)^-1.069
Efficacy treatment	Time/6D

Table 2. Output variables

About the microbial inactivation some studies in literature were already performed (Wang and Toledo, 1986, Malik et al, 2013). With reference to these studies, the Weibull model provided the best fit, and its use was extended to produce a correlation yielding D values over a range from 10 to almost 4000 ppm (D.J. Malik et al, 2013).

In this work, the D parameter was fixed using the Weibull model. In this context, the model accounts for biological variation with respect to inactivation times. The following form of the model was applied here:

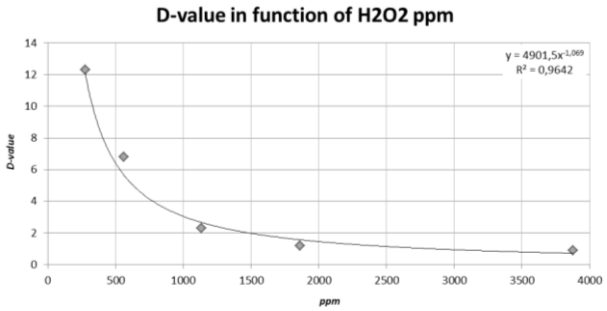
$$\frac{C}{C_0} = 10^{-(\frac{t}{D})^p} \quad (4)$$

where the parameter p is commonly referred to as the 'shape parameter', and D is the decimal reduction value. Wang and Toledo (1986) had examined the inactivation of *B. Subtilis* spores by hydrogen peroxide vapour at concentrations in the range 275-3879 ppm. Table 3 reports D and p values for the Weibull model at high concentration of VHP.

Weibull		
ppm	***p***	***D-value***
275	3.36	12.3
558	1.95	6.8
1131	2.60	2.3
1859	3.33	1.2
3879	3.62	0.9

Table 3. Weibull model inactivation

A power-law regression model describes the hydrogen peroxide concentration dependency of the decimal reduction values as show Graph 1.



Graph 1. D-value in function of H2O2 ppm for the Weibull model

On the basis of these studies it was possible to determinate the D-value in function of the H_2O_2 concentration and to obtain the efficacy treatment parameter.

As already specified, between the input and the output variables, it is necessary to insert the Workbench application node. This part connects the input and output variables. To complete the process flow, the objectives were set. In this work the main objectives to be achieved are two:

- Maximize the efficacy sterilization treatment to exceed six decimal reductions.
- Minimize the costs consumption of H_2O_2.

For the first one, the ratio between the simulation time and the relative D-value was calculated. For the second one, the multiplication among the unit cost of H_2O_2, the mass flow rate of H_2O_2 and the time of the sterilization process was calculated. To complete the data flow, and the entire workflow, ModeFrontier offers many types of modern optimization algorithms, whose specificities are adapted to different optimization strategies.

The correct number of design and the appropriate scheduler for the simulation were individuated in according with the number of the input and output variables and the number of the objectives (Table 4).

DOE method		Optimization algorithm	
Sobol	9 designs	*NSGA-II*	10 generations

Table 4. ModeFrontier scheduler

Sobol DOE method creates sequences of "n-tuples" that fill the "n-space" more uniformly than random sequence. This type of sequence are called quasi-random sequences (Chi et al, 2005). That term is somewhat of a misnomer, since there is nothing random in this algorithm, but filling in a uniform manner the design space.

NSGA-II optimization algorithm is a fast and selective multi-objective (Deb, 2002). A fast non-dominated sorting procedure is implemented. Sorting the individuals of a given population according to the level of non-domination is a complex task: non-dominated sorting algorithms are in general computationally expensive for large population sizes. The adopted solution performs a clever sorting strategy.

Furthermore, NSGA-II implements elitism for multi-objective search, using an elitism-preserving approach. Selectiveness is introduced storing all non-dominated solutions discovered so far, beginning from the initial population. Selectiveness enhances the convergence properties towards the true Pareto-optimal set.

3. RESULTS

3.1 Pareto frontier

ModeFrontier software simulated 90 configurations. In the figure and table below, the Pareto frontier, obtained thanks to all of them, is shown. Also Scatter charts have been created.

A Scatter chart is a two by two quantity chart, it reveals relationships or associations between variables. The values of the variables selected specify the X and Y coordinates of the design.

The first scatter chart (Figure 4) correlates the two objectives: maximize the efficacy sterilization treatment [x] with minimize the costs consumption of H_2O_2 [y].

This case considers two conflicting objectives. From figure 4 it can be observed two different areas: the lower right area shows the maximum in terms of efficacy of treatment but not in terms of the minimum treatment cost. The second area, located in the lower left part of the graph, shows the configurations that reach the minimum cost but not the maximum treatment efficacy. In all the following figures, the green line represents the regression line for the all ID designs.

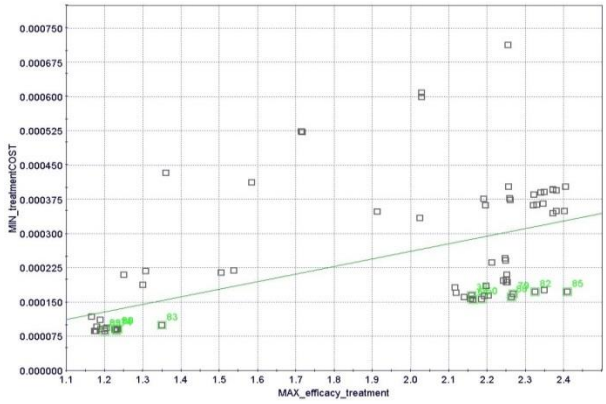


Figure 4. Scatter chart between objectives

The second scatter chart (Figure 5) correlates the average H_2O_2 concentration [x] with the D-value [y].

Increasing the average H_2O_2 concentration, the D-value decrease.

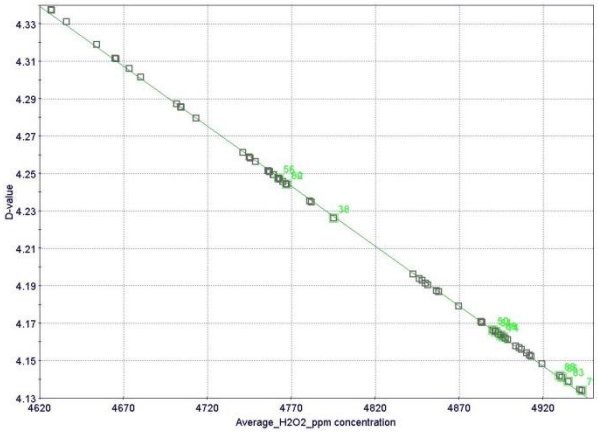


Figure 5. Scatter chats between average H2O2 concentration and D-value

A Scatter 3D chart displays points at the locations specified by the 3-dimensional vectors X, Y, and Z. It reveals relationships or associations between variables.

In the Figure 6, the two objectives and the time of the process were analyzed.

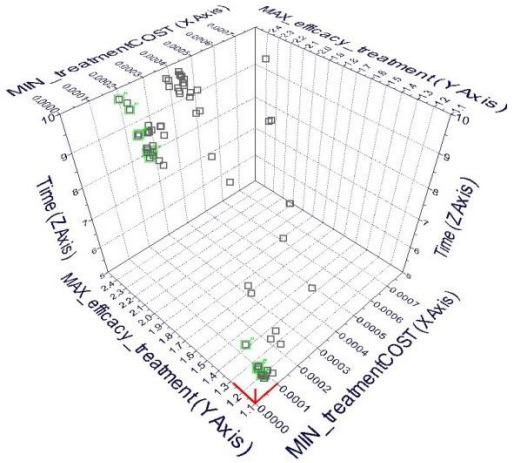


Figure 6. Scatter 3D between two objectives and time

Also the scatter 3D shows the two areas previously described. Furthermore, this 3D graph reports how the two objectives are influenced from the time variable.

The parallel coordinates chart is a method of displaying multivariate data. In this type of chart, a set of parallel axes are drawn for each variable. Then a given set of data is represented by connecting the value of each data on each corresponding axis. The parallel chart is useful to quickly evaluate designs whose variables are in a particular range.

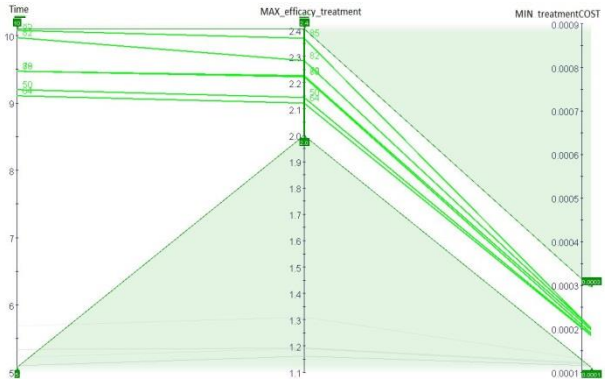


Figure 7. Parallel history of the 13 Pareto designs

Figure 7 shows the Pareto designs with efficacy treatment higher than 2 and treatment cost below 0.00030 € per bottle.

When the sterilizing effect is equal to 1, six decimal reductions are achieved. For some applications this value can be considered a sufficient sterilizing effect. Though, this work purposes to maximize the sterilization level consistently with the other variables. For this case a MCDM method was applied.

MCDM (Multiple Criteria Decision Making) is a post-processing tool which helps the user to make selections of best designs from a family of Pareto solutions. It is extremely useful when dealing with several conflicting objectives.

3.2 Optimal design and MCDM application

The previous results define a clear Pareto frontier and will be used to determine the optimal sterilization process. Among the 90 designs, 11 of them are true Pareto designs, meaning that for these 11 designs one cannot decrease the cost of treatment without decreasing the efficacy of treatment and vice versa. In other words, without performing a multi-objective analysis, one can only treat these designs as equally optimal. Table 5 summarizes the 11 optimal designs including the cost of treatment, the efficacy of treatment, the average H_2O_2 ppm, the D-value, the time and the design ID.

Design ID	Efficacy treatment	Treatment cost	Time	D-value	Average H_2O_2 ppm concentration
50	2.19	1.56E-04	9.10	4.166	4890
56	1.23	0.91E-04	5.23	4.247	4762
64	2.16	1.54E-04	9.01	4.165	4892
65	1.20	0.85E-04	5.00	4.163	4895
74	1.23	0.88E-04	5.13	4.163	4896
79	2.27	1.68E-04	9.37	4.134	4943
80	1.23	0.91E-04	5.23	4.244	4767
82	2.32	1.71E-04	9.87	4.244	4767
83	1.35	0.99E-04	5.59	4.139	4935
85	2.41	1.72E-04	9.98	4.141	4931
88	2.26	1.60E-04	9.37	4.142	4930

Table 5. Resume of 14 optimal designs

These 11 designs are all optimal designs because for each of them it is not possible to reduce treatment cost and increase the sterilization efficacy simultaneously.

A possible way is to apply an MCDM tool that enables one to find the best solution among a set of reasonable alternatives. Table 6 and Figure 8 show the relationships between the variables.

Attribute 1	Type	Weight	Attribute 2
Average H_2O_2 PPM	>	2.0	TreatmentCOST
Average H_2O_2 PPM	=	1.0	Time

Table 6. Relationship between variables

As described before, this case provides the optimum configuration that ensures the optimal sterilizing effect.

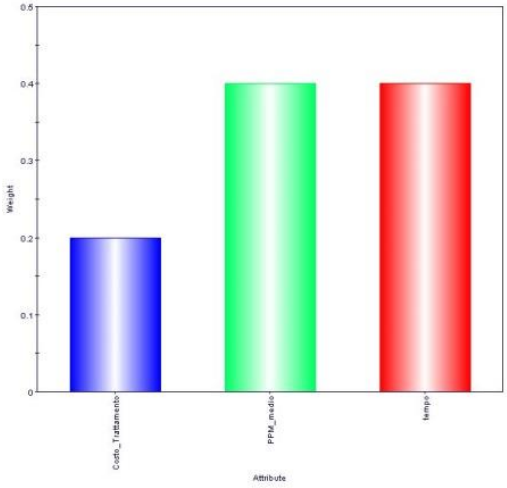


Figure 8. Attributes and weight chart

In respect of the weights previously set, the optimum design can be seen in Figure 9.

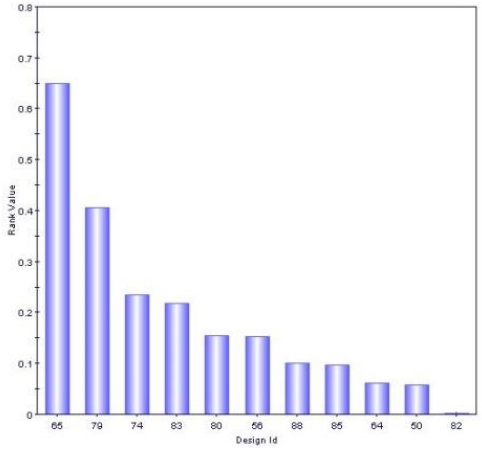


Figure 9. Rank value and Design ID charts

The greatest rank value represents the optimal ID configuration (Table 7).

ID	Treatment cost	Average H_2O_2 ppm concentration	Time	Rank Value
65	0.85E-04	4895	5.00	0.649
79	1.68E-04	4943	9.37	0.406
74	0.88E-04	4896	5.13	0.235
83	0.99E-04	4935	5.57	0.218
80	0.91E-04	4767	5.23	0.154
56	0.91E-04	4762	5.23	0.153
88	1.60E-04	4930	9.37	0.100
85	1.72E-04	4931	9.98	0.096
64	1.54E-04	4892	9.01	0.061
50	1.56E-04	4890	9.10	0.058
82	1.72E-04	4867	9.87	0.002

Table 7. Ranking Value

Among the Pareto frontier, the design 65 represents the best configuration able to reach the optimal treatment efficacy possible according to the other objective and the others variables.

4. CONCLUSIONS

Aseptic filling technology of Spouted Pouch packaging requires a very complex sterilization and rinsing of the packaging before filling.

The aim of this work was to optimize the sterilization process of pouch packaging used in aseptic technology and it has been resolved using a multi-objective optimisation.

ModeFrontier is a multi-objective optimization and design environment which combines a comprehensive process integration platform with sophisticated, optimization algorithms, and powerful post-processing capabilities.

To fully utilize the performance simulation and increase the efficiency of the design, we can introduce optimization algorithms and integrate the simulation program to automatically generate and simulate new designs.

This study goals to optimize the sterilization treatment and its relative cost. A contradiction between these two objectives occurs. By using the MCDM tool, the designer can express his preferences and let the software rank all the optimal designs for selection.

The present study purposes to individuate the optimal sterilization effect able to achieved at least 6 decimal reductions. Decimal reductions pair to 6 means that the sterilizing effect is equal to 1. Basing on the previous considerations, the optimum configuration is the design 65. The parameters of the optimal configuration are: high average H_2O_2 concentration equal to 4895 ppm; short time of the process whose value is 5.00 seconds and low treatment cost equal to 0.85E-04 Euro per bottle.

Future researches could be related to improve the optimization process, adding a SolidWorks node in ModeFrontier in order to change also the nozzle position inside the pouch packaging.

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