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Intelligent Advisor for the Design of Preforms in Stretch Blow Molding

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Abstract

Stretch blow molding is the process of choice for the production of PET containers, for the food and beverage industry as well as the pharmaceutical sector. The stretch blow molding process involves three stages, the reheat stage where previously injection molded preforms are heated to the desired forming temperature distribution, followed by the forming and the solidification stages. The process is a high volume process with costly tooling for both the preform and the container.

The design of the tooling, via virtual technologies is preferable so as to minimize costly tooling reworks. Industry has readily accepted the use of finite element technologies in the prediction of the stretch blow molding process. This acceptance is now generating large amounts of information that are invaluable for future designs. The challenge is now to structure and make use of this information in as efficient a way as possible.

A design database structure has been set up for information representation from past designs, including a design, preform and bottle databases. A process database including results of finite element simulations and the corresponding experimental validations are also integrated into the system. Mathematical methodology has been established to represent preform design. The design database and a series of user-defined heuristic design rules for stretch blow molded containers are used to extract unknown input needed in the design methodology. The heuristic knowledge represents the different product characteristics based on mechanical requirements. They will be converted into fuzzy rules for the data extraction. Those rules and the data extraction will evolve and adapt themselves taking into account new design database, new rules and modified rules. The model inputs are the bottle fill level capacity, bottle diameter, bottle length and bottle transition length, whereas the outputs of the model are the preform shape and weight.

Introduction

PolyEthylene Terephtalate (PET) is a low cost semi-crystalline polymer. It is easy to process due to its strain hardening properties allowing a more uniform deformation. PET is a long molecular polymer chain and the molecules tend to align in the stretched direction, generating molecular orientation that produced the strain hardening effect. This will create anisotropy and non-uniform properties in the final product. Blow ratio is used to describe the stretched level. The axial blow ratio represents the stretch in the length direction, the hoop blow ratio represents the stretch in the circumferential direction and the blow up ratio (BUR) gives an indication of the overall deformation [1] (see figure 1).

The polymer molecular orientation generates residual stresses in the container. Releasing those stresses when filling the bottle with a hot fill product the bottle might deform or rupture. Letting the polymer relaxed while processing the bottle allows the polymer to crystallize reducing residual stresses and molecular orientation [2]. Since PET is a porous material, crystallinity and polymer additive can helps to reduce the oxygen and CO_2 diffusion through the polymer.

Depending of the bottle content, the manufacturing will aim different types of bottle properties. Carbonated soft drink (CSD) bottles have a high molecular orientation to withstand the internal pressure.

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Bottles containing pasteurize product filled at 85°C (hot fill) have a high crystallinity level to resist the filling thermal shock. Bottles containing food have a high crystallinity level to reduce oxygen diffusion. Water bottles have a high molecular orientation to reduce the final weight, since the polymer represents half of the production cost [1].

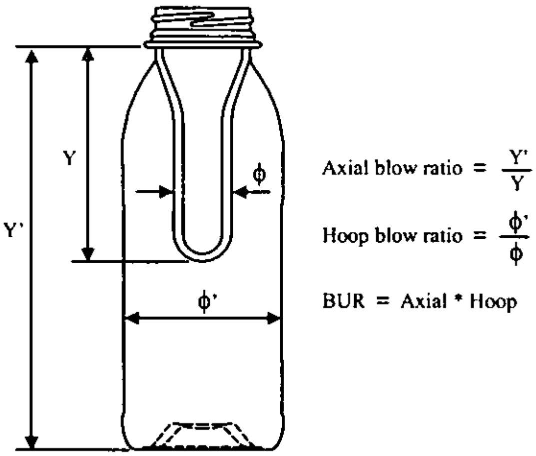

Fig. 1. Blow ratio.

Stretch blow molding design environment

The Industrial Materials Institute (IMI) of the National Research Council of Canada (NRC) with the participation of AMCOR Pet Packaging developed a stretch blow molding design environment software. The aim of this software is to reduce product development time and improve product performance. The design environment software is based on simulation technology (BlowSim software) previously developed at IMI.

BlowSim is a finite element modeling (FEM) solver that simulates the entire stretch blow molding process, from the reheat stage to the solidification stage. BlowSim calculates the temperature, thickness, stress, molecular orientation and crystallinity distribution throughout the entire stretch blow molding process. The molecular orientation and crystallinity distribution are used to evaluate the mechanical properties (Young modulus distribution) of the final product. Knowing the mechanical properties and assuming a Hook's law for the material model, bottle mechanical performance can be determined using BlowSim.

The design environment will help the designer to quickly simulate the stretch blow molding process. Mechanical performances are predicted using the thickness and Young modulus distributions obtained from the process simulation. Three types of load can be simulated: top load, vacuum and pressure. The stress distribution of all the predicted loads is combined and a maximum stress distribution is generated. One optimization module manipulates the final bottle thickness distribution to target user-defined mechanical requirement (yield stress). A second optimization module manipulates the processing conditions to target the final bottle thickness distribution. Finally, a third optimization module finds the parameterized preform geometry to target a final bottle thickness distribution.

Initial preform design

The preform geometry and processing conditions are usually unknown when designing a new bottle. Initial designs have a significant influence on the development time and the final design, so it is important to have a good initial design. Using an existing preform may decrease development and tooling cost while designing a new preform might reduce the weight and improve the final bottle performance. Using virtual technologies allow to rapidly evaluate both options. The design environment includes a module that rapidly proposes initial preform geometry, also called Preform Design Advisor (PDA). The PDA is the subject of this paper.

Preform Design

The complete preform design mathematical methodology will not be discussed herein since this information is confidential and belongs the AMCOR Pet Packaging Company. A summary of the preform design rules used in this work can be simplified as:

1. Select the design weight and blow ratio (hoop and axial) based on the bottle geometry, mechanical and client requirement.
2. Calculate the preform length and diameter using the bottle geometry and blow ratios.
3. Set the preform thickness by distributing the weight along the preform.

Preform Design Problematic

Some design input parameters (weight, blow ratios, etc) are usually unknown. They are usually chosen based on designer and company knowledge and experience. This soft data is often not or partly considered because the result depends on how the designer uses the data. Also, it is usually believed that the soft data is hard to use and hard to extract information from it.

The designer and company experience may be encapsulated in past design database. Using the designer knowledge of the complex relationship between different parameters, a search and extrapolation from the design database can provide the needed data.

Preform Design Criteria

The designer can let the PDA extract all the needed data from the database or can fix some inputs. Designer can also impose criteria on inputs or on the search and extrapolation. If the designer fixes inputs, they will not be extracted from the database. The designer can restrict the range of some inputs as well. The data search and extrapolation can be restricted to a specified product type and specified finish.

Database

Past designs are structured in a design database as illustrated in Figure 2. This structure is set up to avoid information duplication and allow maximum efficiency.

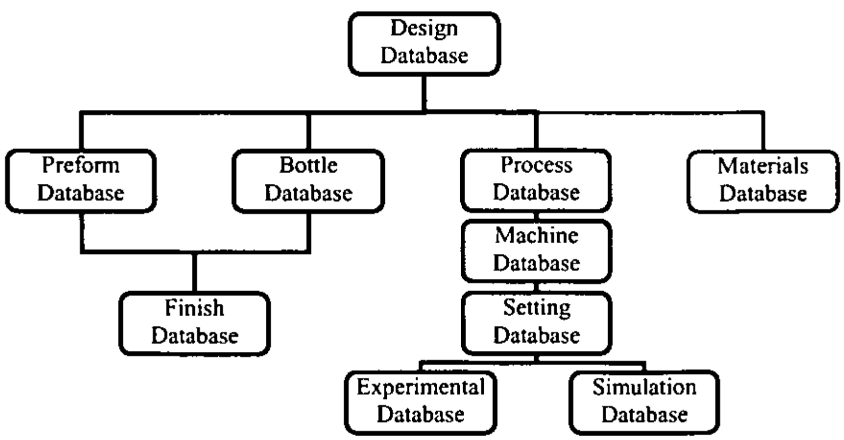

Fig. 2. Past design database structure.

The design database associates the preform and bottle geometries and includes the processing information. The preform, bottle and finish databases contain the parameterized geometries, allowing to represent the geometry in a design perspective and to easily modified them. The process database includes an indication of the design fitness, represented by the *design reliability level*. This parameter lets the user defined the quality of a design, usually based on the satisfaction of the mechanical requirement and the weight. The simulation and experimental databases are very helpful to determine this parameter.

Design database are regrouped in design lists. The design lists allow regrouping designs that have similar design philosophy. Those philosophies can be based on the bottle product type, mechanical loads or requirements, processing conditions, bottle geometry characteristics, etc. Judiciously grouping designs allow the list to inherit the design properties that satisfy a mechanical performance and client requirements.

Data extraction

In a company, numerous past designs are usually available. However, a large number may be out of date, by a design perspective, and a large variety of client requirements can be found. For a specified design type, the number of relevant past designs is often reduced between 5 and 50.

Extrapolation methodologies could be used to extract the needed information from the database. However traditional extrapolation methodologies cannot take into account complex relationship between parameters. Some soft computing techniques can be used to represent or get the complex relationship from many inputs and outputs parameters [3]. The combination of soft computing techniques and databases may provide the needed data.

Using the design list of past designs and the knowledge of the complex parameters relationship, a fuzzy system can be built. The fuzzy rules represent the designer knowledge of the parameters relationship. The fuzzy inputs are the bottle geometry parameters. The fuzzy outputs are the unknown design input parameters.

More information could by extracted from the fuzzy system (fuzzy output). Additional design features could also be extracted from the databases, like the preform transition radii and preform draft angles (see figure 3).

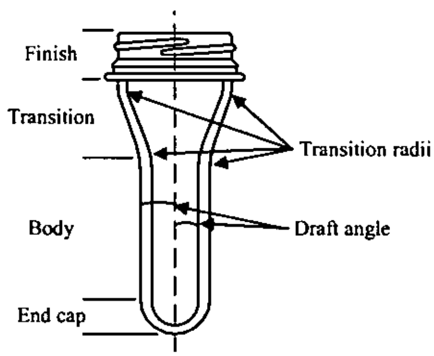

Fig. 3. Preform nomenclature.

Preform transition radii help having a gradual thickness transition in the preform to avoid demarcation on the final bottle. The preform draft angles help demolding the preform when ejected. Those additional features can be added after the initial design so they do not change the basic preform design rather than improving it. Consequently those features can be based on the bottle geometry and the preform basic geometry.

To take into account the designer knowledge of the parameters relationship, the PDA allows the designer to define the extrapolation rules. The rules are weighted to allow the designer to balance their influence. The PDA includes a default extrapolation rule, if an unknown design input parameter is removed from all the rules, the module will reincorporate this parameter in the default rule or add the default rule. Those extrapolation rules are converted into fuzzy rules before the data extraction is made. The fuzzy rules are weighted taking into account the extrapolation rules weight and the database *design reliability level*.

The fuzzy inputs are defined by the extrapolation rules. The fuzzy inputs can be bottle and preform geometrical parameters, *bottle fill level capacity*, *bottle diameter*, *bottle length*, etc. The fuzzy inputs can also be ratio of those parameters, *bottle diameter* divided by *bottle length* multiply by *bottle fill level capacity*. The fuzzy input membership function may be wildly spread or regrouped. To ensure that the parameter domain is completely defined, Gauss membership functions are used for the fuzzy inputs.

The user's define extrapolation rules are defined as the following:
The *Design weight* and *axial blow ratio* depend on the *bottle fill level capacity* with a weight of *100*.
The *axial blow ratio* depends on the *bottle fill level capacity* divided by the *bottle length* with a weight of *65*.

Domain Balance

The extrapolation rule, the criteria and the design list may change for every design; the fuzzy system must be set no matter the user inputs.

Using uniform standard deviation for the fuzzy input membership function may cause problem. First some part of the domain may not be defined, where the sum of the membership functions is less then 0.05. Secondly, if all the membership functions are regrouped, the domain may shift toward the regrouped values.

To set the standard deviation of the fuzzy input membership function, three conditions must be satisfied:

1. At every inner membership function average value, the influence of all the other membership function must balance themselves:

$$\sum_{i=2}^{n-1}\sum_{j=1}^{n} MF_j(\mu_i)\times(\mu_i-\mu_j)=0 \quad 1.$$

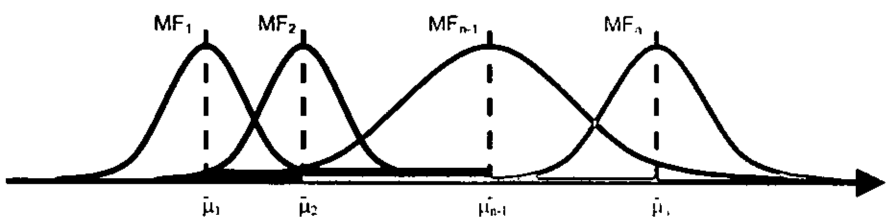

Fig. 4. First condition to set the fuzzy input membership standard deviation.

2. At any point between the two extreme membership function average value, the sum of all the membership functions evaluated at this point must be greater then 0.5:

$$\forall x \mid \mu_1 < x < \mu_n, \sum_{i=1}^{n} MF_i(x) \geq 0.5 \quad 2.$$

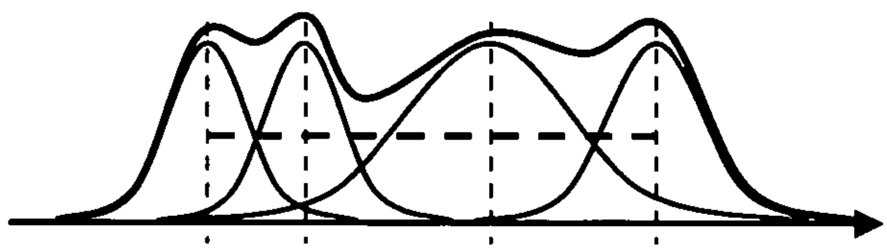

Fig. 5. Second condition to set the fuzzy input membership standard deviation.

3. At any point smaller then the second membership function average value or greater then the second last membership function average value, the sum of all the membership function evaluated at this point must be smaller then 1.0:

$$\forall x \mid x < \mu_2 \vee x > \mu_{n-1}, \sum_{i=1}^{n} MF_i(x) \leq 1.0 \qquad 3.$$

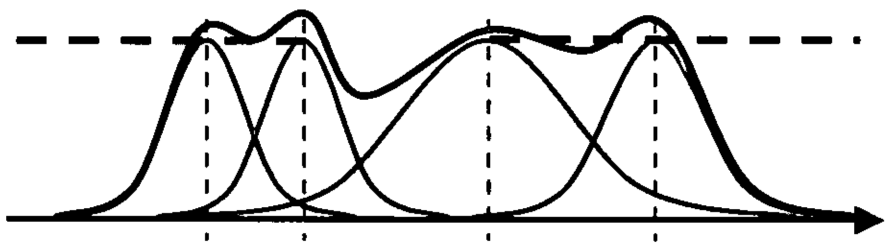

Fig. 6. Third condition to set the fuzzy input membership standard deviation.

Where n is the number of membership function, μ_i is the membership function i average value and $MF_i(x)$ is the membership function i evaluated at x.

The third condition ensures that extrapolation outside the two extreme membership function average value is mostly made using the extreme membership function. If the third condition is not used, the extreme membership function standard deviations would tend to be minimized since they are not taking into account in the first condition.

To guarantee the repeatability of the design, a global optimum of the standard deviation values distribution must be found. Genetic algorithm (GA) [4] is used to find the distribution of the input membership function standard deviation. Since the problem to solve is difficult and that GA does not guaranty to find the global optimum, special features are included in the GA: generation overlap, macro GA, forced macro GA, niching, particular convergence criteria and civilization overlap.

The generation overlap lets a given number of the best chromosomes from one generation to be transferred directly to the next generation. If generation overlap is not used the algorithm is no able to solve the problem.

Macro GA is performed when the convergence criteria are not reached and the population distribution congregated. The Macro GA keeps the overlap population and randomly recreates the rest of the population. This is done to get out of local optimum.

If the convergence criteria are not reached for a consecutive number of generations after a macro GA was done, forced micro GA is made which randomly recreates the population keeping the overlap population.

Niching also help to avoid local optimum by averaging the fitness value with the level of scattering.

Three convergence criteria are used:

- the best chromosome does not change for a consecutive number of generation;
- the overlap population average fitness value decreases less then a given percentage for a consecutive number of generation;
- the overlap population fitness standard deviation decreases less then a given percentage for a consecutive number of generation.

The GA objective function is formulated so the global optimum fitness value is known. If the global optimum is not reached after the first GA, a second GA is performed using a number of the best chromosomes from the previous GA. This is called the civilization overlap and the number of chromosomes transfer to the next civilization is usually less then half then in the generation overlap.

A global optimum is usually found within three civilizations if the maximal fitness value exists. Figure 7 shows an example where the maximal fitness value does not exist. If the global optimum is not found, the optimum distribution obtain will be used and a warning message will inform the designer.

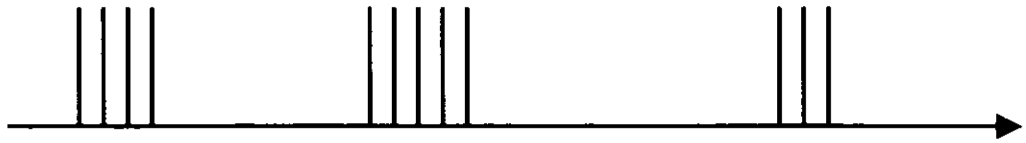

Fig. 7. Representation of a bad fuzzy input distribution.

Test case

3 CSD bottles with fill level capacity of 355 *ml*, 600 *ml* and 1.5 *l* were designed using the preform design advisor (PDA) and past CSD designs. To understand the design list influence, past CSD designs are regrouped in 3 categories: sparkling water bottles, silhouette bottles and light CSD bottles.

- The sparkling water bottles include designs from 500 *ml* to 1.5 *l*.
- The silhouette bottles are thicker bottles so they do not deform with the internal pressure, they include designs from 475 *ml* to 750 *ml*.
- The light CSD bottles represent the rest of CSD bottles and include designs from 250 *ml* to 3 *l*.

Using the previous groups, four different design lists are used in the PDA:

1. all the CSD designs (sparkling water bottles, silhouette bottles and light CSD bottles);
2. silhouette bottles;
3. light CSD bottles;
4. silhouette bottles and light CSD bottles.

No criteria were used. So all the unknown design input parameters were extracted from the design list. To observe the repeatability of the design methodology, each design was performed 10 times. Tables 1 to 3 resume the results for the 3 bottles studied. The results are compared with the design obtain using the completed CSD design list (all).

Table 1: Proposed preform geometry for the 355 *ml* bottle.

		Weight (g)	Length (mm)	Body Thickness (mm)
All	average	μ_W	μ_L	μ_T
	std	0.1	0.3	0.06
	min	μ_W - 0.1	μ_L - 0.3	μ_T - 0.1
	max	μ_W + 0.1	μ_L + 0.6	μ_T + 0.05
Silhouette	average	μ_W + 3.4	μ_L - 6.0	μ_T + 1.9
	std	0.1	0.49	0.14
	min	μ_W + 3.4	μ_L - 6.20	μ_T + 1.6
	max	μ_W + 3.5	μ_L - 5.1	μ_T + 2.0
Light CSD	average	μ_W + 1.7	μ_L + 12.0	μ_T - 0.4
	std	0.05	0.08	0.02
	min	μ_W + 1.6	μ_L + 11.9	μ_T - 0.4
	max	μ_W + 1.7	μ_L + 12.1	μ_T - 0.4
Silhouette + Light CSD	average	μ_W + 0.9	μ_L - 1.3	μ_T + 0.2
	std	0.4	0.16	0.17
	min	μ_W + 0.6	μ_L - 1.5	μ_T + 0.02
	max	μ_W + 1.6	μ_L - 1.1	μ_T + 0.4

Table 2: Proposed preform geometry for the 600 *ml* bottle

	Weight (g)	Length (mm)	Body Thickness (mm)
All	μ_W	μ_L	μ_T
Silhouette	$\mu_W + 0.8$	$\mu_L + 0.6$	$\mu_T + 0.2$
Light CSD	$\mu_W + 3.2$	$\mu_L + 21.1$	$\mu_T + 0.1$
Silhouette + Light CSD	$\mu_W + 1.1$	$\mu_L + 3.6$	$\mu_T + 0.2$

Table 3: Proposed preform geometry for the 1.5 *l* bottle

	Weight (g)	Length (mm)	Body Thickness (mm)
All	μ_W	μ_L	μ_T
Silhouette	$\mu_W - 12.0$	$\mu_L + 0.5$	$\mu_T - 1.7$
Light CSD	$\mu_W - 1.4$	$\mu_L + 20.2$	$\mu_T - 0.4$
Silhouette + Light CSD	$\mu_W - 1.5$	$\mu_L + 20.2$	$\mu_T - 0.4$

Results and Discussion

The small standard deviation and value ranges indicate that the results are very repeatable. The domain balance always converges to the same optimum solution. Moreover, 20 different distributions were tested 500 times and they always converge to the same solution within a numerical precision.

For the 355 *ml* and 600 *ml* bottles, lighter and shorter preforms were proposed when using the complete design list (All). This was expected since this list is the only one taking into account the sparkling water design. Longer preforms were proposed using the light CSD list, this was also expected because those designs have a higher hoop blow ratio to maximize the circumferential strain hardening properties.

The proposed preforms for the 600 *ml* bottle using the silhouette bottle list should be heavier than the one proposed using the light CSD bottle list. This is not the case because the light CSD bottle list is composed of some bottles between 250 *ml* to 450 *ml* and the majority of bottles around 1 *l*, 2 *l* and 3 *l*. A heavier preform is proposed because the extraction is pulled toward the design with higher fill level capacity to compensate the hole in the domain. This was expected since, in the GA, the maximum fitness value is never reached when balancing the light CSD bottle list.

For the 1.5 *l* bottle, the proposed preforms using the silhouette bottles list is 12 *g* lighter then ones proposed using the other lists. The silhouette bottle list domain of validity is from 400 *ml* to 800 *ml* and since the weight is directly extracted, the extraction gives the value at 800 *ml*. However the length is calculated using the axial blow ratio, the length is extrapolated at 1.5 *l* using the axial blow ratio at 800 *ml*. The design philosophy from the weight is not respected although it is respected for the preform length.

This has showed that the proposed methodology for the data extraction is reproducible. It has also been shown that the past design lists have a big influence on extracted data. If the lists are badly built, the extracted data may be inaccurate and may not represent adequately the list design philosophies.

Remarks and Conclusion

In this work, a preform design methodology has been presented. The methodology is based on design mathematical rules and extrapolation techniques using soft computing for unknown inputs. Using a list of past designs having the same design philosophy and extrapolation rules, the unknown or missing data are extracted and preform geometry is proposed. The past designs and extrapolation rules represent the designer and company knowledge and experience. New designs may be added to the design list and extrapolation rules can be modified and added to the module allowing it to evolve and adapts with time. It is important to judiciously group the preform so the preform inherits the satisfaction on the client requirements.

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