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New Modelling and Process Optimisation Approach for the False-Twist Texturing of Polyester

Abstract
After the wave of ISO 9000 certification, a large number of enterprises started to accumulate a great amount of data regarding their processes. False-twist texturing plants used these data to set up a process and improve their operations. This article shows that data mining, partial least squares modelling and genetic algorithm optimisation can provide further use for these data to benefit the company in many areas, such as setting up adequate process parameters without requiring an expert to do so, providing the customer with the requirements that will fulfill his needs, simplifying machine changes, and reducing lot changes. The results show that the model and optimisation structure put together can find multiple solutions for machine parameters by providing the multiple product properties or quality levels desired. The prediction of yarn properties, such as linear density (Dtex), elongation, tenacity and boiled water shrinkage were made with R^2 between 0.80 and 0.99.

Key words: *polyester filament, texturing, false twist, multivariate statistics, optimisation, partial least squares, genetic algorithm.*

Introduction

At the SYFA (Synthetic Yarn and Fibre Association) 2007 summer conference [1], PCI (Petrochemical Consultants International) Fibres reported 10.6 kg/capita of fibre consumption in 2006 as an average worldwide, with polyester filament yarn having a share of 23% of the global fibre market. In the global synthetic market, polyester represents 71% of the market - nearly 28 million tons per year as far as the 74% average capacity utilisation is considered. In this context, after spinning, false-twist texturing remains the main filament converting process currently used worldwide. The false-twist texturing process uses a POY (partial oriented yarn) as the raw material to obtain the yarn properties desired. The required features of the respective POY will be achieved by properly adjusting the texturing machine parameters. To understand the relationships and interactions in the process, some studies have been carried out.

Based on the fundamentals of mechanics [2], a new twist theory for friction discs is presented using experimental data to prove it. Using the principle of energy and mass conservation, elongation curve analyses as well as the twist structure [3] describe how to predict yarn properties using filament data. A mathematic model is proposed that could predict the elongation, tenacity and initial modulus. Using design of experiments (DOE) [4] for microfibre, three raw material types were textured focusing on 4 factors (draw ratio, disc surface speed to yarn speed ratio (D/Y), first heater temperature and heater contact time). The responses analysed were tensile properties, crimp characteristics, dye uptake, broken filaments, and tight spots. The Lagrange approach was used [5] to simulate the false twist texturing process. Another DOE is presented [6] to demonstrate the influence of temperature in the first heater, disc space, draw ratio and D/Y on the yarn properties. The Box-Behnken DOE design with 3 levels was used, allowing 27 experiments to verify the relationships, which also showed relevant interactions.

The majority of the articles previously mentioned only regard the false twist texturing of polyester and do not utilise any multivariate approach, such as partial least squares. This article fills that gap by presenting its functionality.

In a texturing manufacturing environment, optimisation takes place daily through causal models built in designed experiments, as mentioned previously, that relate the independent effects of all factors that can be changed in the process with the response variables of interest. However, the false twist process is extremely complex and contains a vast number of manipulated factors, of which the majority are highly correlated within the process or follow operational constraints. For example, yarn shrinkage correlates with the linear density (Dtex), Dtex per filament, temperatures and production speeds; in such cases complete causal models are not easily obtained. Considering that ISO 9000:2000 (as well as older versions) brought discipline to companies as well as guidelines to store large quantities of data, a great and significant amount of quality data are available for a range of operational working conditions of the process. These data can provide the means to build one restricted causal model that shows how process groups or raw material factors can impact product quality in the form of subspaces of the original factors. This can be considered as being a big DOE developed over time in the manufacturing environment. Linear or non linear latent variable models built using partial least squares are ideal for such a reality. See [7] for a similar approach to extrusion.

In this article, a methodology is proposed for process development and control based on optimisations of subspaces as defined by latent variables built with existing and available data. Models with linear latent variables are developed and an optimization strategy using genetic algorithms is implemented to resolve important goals of product development, process control, planning flexibility and reduction in machine setup times. A PLS (partial least square) methodology using Minitab software to model the process and a genetic algorithm using Excel solver to optimize it were applied to the false twist polyester texturing process, which proved to be extremely effective in determining process conditions that yield the specific quality goals desired. This reduces the development time required to obtain the final product as well as its variability, due to not optimised parameters.

Modelling and optimisation using historical data

In the development and/or optimisation of chemical textile processes, it is essential to identify which process variables have an effect on the final product quality as well as their variability throughout the many process stages. If a dynamic fundamental model of the process is available, the company can use it to develop new products as well as optimise or control the process against different raw material variations in the environment or structural conditions. Alternatively, an empirical model that estimates the causal effects of adjustable, process and raw material variables in the quality process can be obtained by planned experiments. These models can be used in a similar way (within the working region defined) to optimise or control the process [8]. However, for the majority of complex processes, fundamental models that consider all variables are not available, and for processes consisting of vast numbers of variables (any chemical or synthetic process can reach such a level), with highly correlated variables that can not be independently manipulated, it becomes extremely difficult to obtain empirical models that will represent the causal relationships that exist in the process within the operational constraints, cost constraints or even time to market constraints.

__Table 1.__ Correlation and R-sq between actual and calculated data using mechanics fundamentals equations.

Calculated	Actual	Correlation	R-sq, %
YC1	Y1	0.936	87.5
YC2	Y2	0.901	81.2
YC3	Y3	0.701	48.6
YC4	Y4	0.998	99.6
YC5	Y5	0.774	59.7
YC6	Y6	0.443	19.0
YC7	Y7	0.720	51.7

With the broadening of process standardisation and ISO (International Standardisation Organisation) standard utilisation, a mindset for using historical data was created, whose importance and utilisation is increasing daily. Primarily, the data were used to control and trace information simply. Currently, the data are identified as potentially useful information through which an immeasurable quantity of knowledge can be generated if adequate data analysis has taken place.

New approach for the modelling

In January 2003 at the TYAA (Textured Yarn American Association), currently SYFA, winter conference in Charlotte some works regarding texturing and spinning modelling were presented. Both works used the fundamentals of mechanics to achieve the modelling. As [9] stated in 2002, like most developments on the mechanical side of the textile industry, inventions and developments in yarn texturing have not come as a rational sequence from basic science, through engineering calculations to practical implementation. Empirical advance based on intuitive understanding has been the norm. This is not to say that academic research has been wasted. As the science of any aspect of the subject is clarified, this feeds into the qualitative understanding of those concerned with practical operations. The mathematics may be ignored, but the ideas enter the technical consciousness.

From unpublished works, which are used by leading manufacturing industries, such as Unifi Inc and Milliken, models are available to explain a causal relationship sufficiently to allow specialists to predict yarn properties and process parameters. No optimisation for the false twist texturing process has yet been proposed in literature or by manufacturing that is known.

This article proposes a model that can improve responses and therefore enable the optimisation of the process.

Internal modelling by Unifi Inc using the fundamentals of mechanics can provide correlation numbers, given in ***Table 1***, between the values calculated (YC1 till 7) and the actual ones (Y1 till 7). Another way of verifying this relationship is the R^2 (R-sq) between the same values calculated and the actual ones.

From the comparison shown in ***Table 1***, we can observe that some predictions need to be improved. The model previously mentioned (can not be detailed due to proprietary reasons) utilises intermediate calculus allowing the equation to be built. The intermediate equations come from univariate statistics where only significant factors are included in

__Table 2.__ Linear regression using all factors to predict Y1, VIF > 5 shows this is not adequate.

Predictor	Coef SE	Coef	T	P	VIF
Constant	-146.00	1127.00	-0.13	0.898	
X1	+7.96	30.82	+0.26	0.798	4.238
X2	-0.64	1.23	-0.51	0.610	41.944
X3	-3.69	2.15	-1.72	0.093	4.568
X4	-3.40	110.90	-0.03	0.976	2.522
X5	+1.10	3.29	+0.34	0.739	43.432
X6	+5.16	5.64	+0.91	0.366	5.191
X7	+269.50	182.80	+1.47	0.149	9.102
X8	-110.13	23.22	-4.74	0.000	1.836
X9	+66.13	76.17	+0.87	0.391	4.248
X10	-0.11	0.17	-0.68	0.500	2.514
X11	+435.10	433.00	+1.00	0.321	3.375
X12	-290.90	211.10	-1.38	0.176	3.024
X13	+11.73	8.28	+1.42	0.164	2.853

the equation. Therefore the quality of the intermediate equations will influence the final calculations of the data predicted . To illustrate this, an example could be taken to predict the shrinkage of yarn, in which an equation is needed to predict the linear density, the yarn temperature at the exit of the heater, the orientation level, the amount of twist, and the residence time in the fixation heater. These would be some examples of intermediate calculation due to the choice of using the fundamentals of mechanics; for a multivariate approach this is not necessary.

In univariate regression the VIF (Variance Inflation Factor) is recommended to be under 5, but as higher number factors are introduced some factors will appear where this number will pass the threshold of 5, for example to calculate Y1 if all predictors are considered. VIF results can be seen in ***Table 2***. This table demonstrates that univariate regression requires fewer predictors or that an multivariate approach needs to be considered.

A multivariate approach using PLS

Further correlation analysis can demonstrate that multicolinearity is present within the X variables (the predictors) and Y variables (the dependents). A high multicolineraty is not desirable as this indicates redundant measurements and reduced statistical efficiency, which is a reasonable justification to use multiple regressions. Multiple regression is a statistical technique that can be used to analyse the relationship between the one unique variable dependent (criteria) and various independent variables (predictors). The goal of a multiple regression is the use of independent variables whose values are known to predict the those of selected dependent variables. Each independent variable is weighted by the regression analyses procedure to guarantee maximum prediction for the independent variables. [10]

In the texturing process there is correlation between the factors and responses, which justifies the utilisation of partial least squares regression. This can also be found as a projection of latent structures in the literature. A model can then be built to predict the real values using manipulated factors.

For PLS modelling the same group of predictors are used for each predicted variable. This property is the result of the multivariate approach of PLS, therefore one variable can not be studied separately from the group without changing the entire group. The algorithm used is NIPALS. This method of regression equation construction attracted great attention in the 1990's (see [11] for more details).

Regression using PLS is an extension of the multiple linear regression model and can be represented as:

$$Y = b_0 + b_1X_1 + \\ + b_2X_2 + ... + b_pX_p \quad (1)$$

In the equation 1, b_0 is the regression coefficient for the interceptor, and values b_i are regression coefficients (for variables from 1 to p) calculated from the data. The variables predicted will be from Y_1 to Y_i according to the study; in this article they were from 1 to 7.

Regression by PLS amplifies the multiple linear regression without imposing restrictions by discriminant analysis, regression by principal components, and canonical correlation. In PLS regression the prediction functions are represented by factors extracted from the matrix ***Y'XX'Y.*** The numbers of prediction functions possible that can be extracted will typically exceed the maximum variables *Y* and *X*.

In summary, PLS regression is the less restrictive of the various multivariate extensions of multiple linear regressions. This flexibility allows PLS to be used in situations where the multivariate method is severely limited, as when fewer observations than the predictor's variables exist (i.e., few answers and large input data). Furthermore, PLS regression can be used as an exploratory analysis to select adequate independent variables and identify outliers before the classical linear regression.

PLS regressions are used in various fields, such as chemistry, economics, medicine, psychology, and pharmacology where predictive modelling, specially with large numbers of predictors, is necessary. Especially in chemiometry has PLS regression been the standard tool for linear relationship modelling between multivariate measurements. [12]

The data base

Considering that a theoretical robust model is not available to be used for modelling and further optimisation, it was therefore necessary to build an empirical model for control and optimisation purposes and to design an experiment with all the raw material variables and all the manipulated process variables to be able to establish the causal relationship that needs to be modelled. For this study a limited raw material type was used because the methodology can be used to any other desired; a DOE is an

Table 3. *Description of the dependent variables used in this study.*

Variables (Matrix X)	Predictor	Lower	Upper
POY, Dtex	X1	128.00	567.00
Filaments	X2	34.00	136.00
Draw force, cN	X3	40.00	212.00
Elongation, %	X4	101.00	138.00
Production speed, m/min	X5	400.00	950.00
Draw Ratio	X6	1.50	1.87
D/Y	X7	1.52	2.15
Overfeed 2, %	X8	0.00	8.90
Overfeed 3, %	X9	0.00	8.90
Overfeed 4, %	X10	0.00	8.90
Short heater temperature, °C	X11	200.00	550.00
Long heater temperature, °C	X12	200.00	550.00
Secondary heater temperature, °C	X13	0.00	240.00

Table 4. *Description of the independent variables used in this study.*

Variables (Matrix Y)	Response
T1, g	Y1
T2, g	Y2
Actual surge speed, m/min	Y3
Dtex/ply	Y4
Elongation, %	Y5
Tenacity, cN/tex	Y6
Boiled water shrinkage, %	Y7

expensive option due to the high number of variables, cost and time constraints and the fact that the manipulated data were highly correlated. The correlations within X_1 to X_{13} as well as the correlations from Y_1 to Y_7 can be calculated using any statistical software.

The data were collected at the T5 plant of Unifi Inc during production, start-ups, trials, and sample production when technicians manipulated the variables to attain certain properties or quality levels desired. This educated trial and error process coordinated by the technical group is in reality a false DOE at multiple combinations of the manipulated variables, allowing causal modelling in restricted areas which are common or not concern the production. The partial least square method (latent variables) is excellent to built a model for these types of data. The resulting models do not provide independent information for all process variables but will provide causal effect models in a reduced subspace of the operational region sufficient to meet expectations or normal operational needs.

The dependent variables used are described in ***Table 3***. The data matrix used has 303 lines (observations), each line means a different product made with different process parameters. The raw material was semi-dull round polyester. The group formed from X_1 to X_4 is the raw material block, a number of other variables could be considered. The other manipulated variables, X_5 to X_{13}, are some of the most important information regarding process conditions. The region used in each variable is broad and can adequately represent a texturing plant today. The resulting matrix X is 13 × 303; ***Table 3*** also details its actual range.

The response matrix Y (independent variables) is given in ***Table 4***, Y_1 to Y_3 represent important process condition information, and Y_4 to Y_7 are physical properties of the product. The resulting matrix Y is 7 × 303. The dependent and independent variables form a complete matrix that will be used for partial least squares analysis.

The notation used for the modelling and analysis is represented in matrix form. Without losing generalisation, a process parameter can be referred to as a process variable, and a mechanical property as a quality variable. If X_n denotes the process observations from 1 to 303, then X_{nm}, being m from 1 to 13, denotes the individual process variable, and if Y_n denotes the n^{th} quality variable observed, then Y_{nr}, being r from 1 to 7, denotes the individual quality variable.

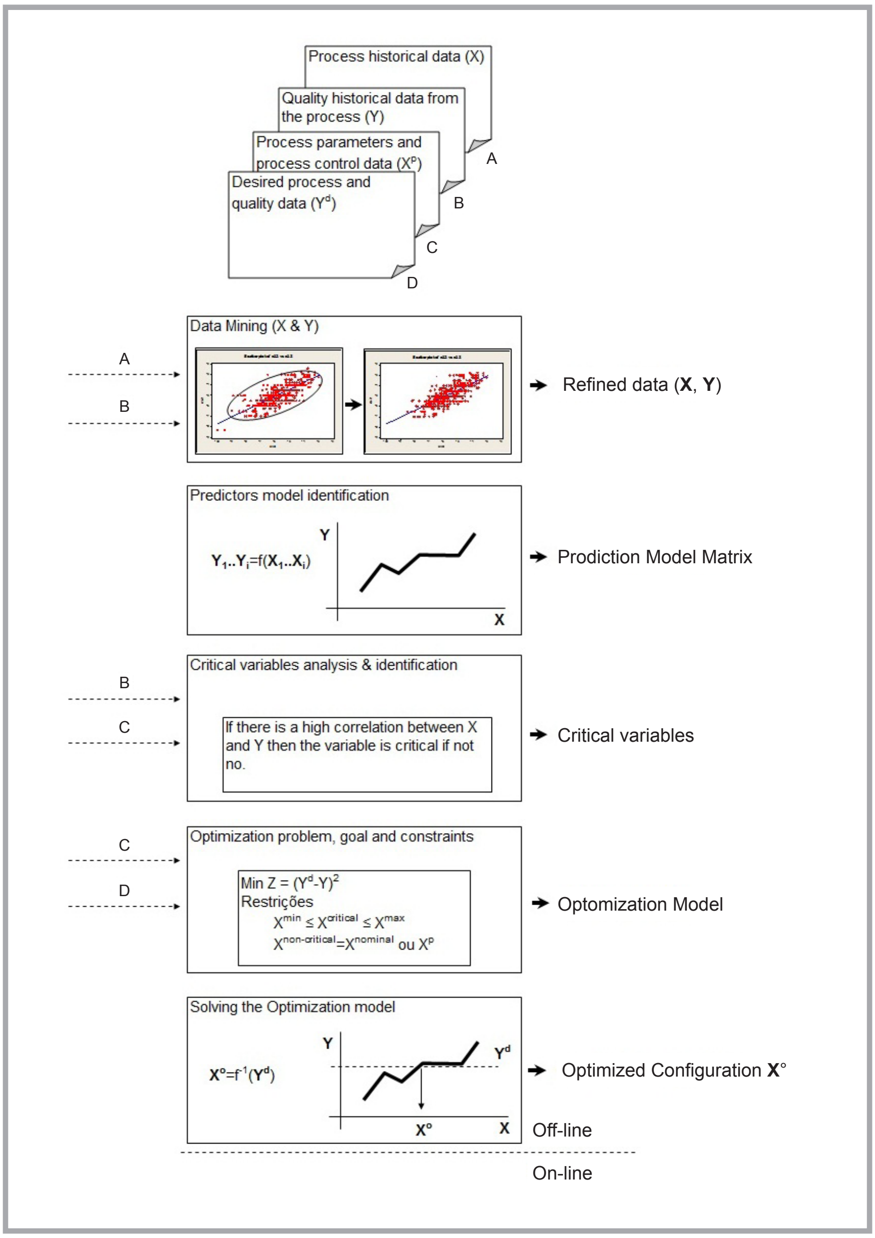

Figure 1. *Information follow steps; adapted from [14].*

Modeling methodology

Figure 1 shows the information flow steps used to achieve modelling and optimisation using historical data. It is evident that all the analysis process occurred offline, which confirms the amount of la-

Table 5. *Compare results of a multivariate versus univariate regression approach.*

Calculated PLS	Actual	Multivariate Regression		Univariate Regression	
		Correlation	R-Sq	Correlation	R-Sq
YP1	Y1	0.95	89.8	0.94	87.5
YP2	Y2	0.93	85.5	0.90	81.2
YP3	Y3	0.83	67.7	0.70	48.6
YP4	Y4	0.99	97.3	0.99	99.6
YP5	Y5	0.87	74.7	0.77	59.7
YP6	Y6	0.80	64.6	0.44	19.0
YP7	Y7	0.86	73.3	0.72	51.7

tent knowledge that exists in a good quality data base.

A factor analysis showed 5 principal components that contain the majority of information regarding the 13 predictor variables, which explains the potential of PLS to reduce dimensionality. According to [10], when a big amount of data is transformed into factors, the combinations of variables are placed in order of variance explanation, from which the researcher can choose the number of factors to utilise; the "scree plot" can help to make this decision. Is this study 10 factors were used for the model acquisition.

To generate the PLS regression model, a Minitab 15 was used. All the Y's predicted were significant with a high R-sq (over 0.65). ***Table 5*** details the improvement in correlation using the PLS approach, in which all the values calculated improved over the univariate approach. It also shows the R-sq determined using the PLS approach, with all the results showing an improvement.

In the face of the remarkable results shown in ***Table 5***, PLS must be recommended to be used in the texturing process for regression purposes. The results also indicate that modelling in the industry can be utilised more frequently than it is today and verify that the statistical tools available have much to offer for continuous process improvement, a fact that it is in the minds of all people in industry today.

Since the model is complete and recognised as being robust, optimisation can be applied.

Evolutionary or genetic algorithm

Evolutionary algorithms are procedures for optimising, learning, and modelling based on the principles of natural evolution. These formal systems tend to be isomorphic with natural evolution. They were created for two purposes: to understand natural evolution better and to help apply the principles of natural evolution to solve various tasks [13].

This technique utilises a solution population instead of one unique point in gradient methods of optimisation. Based on the law of natural selection, the solution that satisfies the objective function will "survive" the mutations and combinations.

This is a global optimisation method that can have different areas of application, such as lay-out projects, machine condition determination, constructions projects, system parameter estimation, and process parameter optimisation. [14]

The evolutionary algorithm finds solutions through a chromosome group - in each generation a new population is generated through genetic operations such as birth, crossover, mutation and elitism.

A random population is first created using a specified probability. The breeding algorithm is also probabilistic, and therefore the accumulated sum of values of the fitness function of each chromosome is normalised to a sum of 1. The new population is then generated randomly, following the probabilities established according to the frequency accumulated. The procedure is similar to the Monte Carlo simulation. The optimisation algorithm used was Excel added to "evolutionary solver".

Multivariate Optimisation

For the optimisation the genetic algorithm was selected because it is evolutionary, similar to human behaviour in the trial and error attempts to improve a process, for example.

The competitive environment that enterprises are today, where extensive research and development of new products and processes is realised to improve the quality levels desired, can change little or considerably as result of R&D activities. The challenge is to implement changes and/ or improvements without great or unnecessary investment.

As in the texturing process, many variables exist, some of which are determined and or specified with respect to the raw material, whereas other qualitative variables are specified by the customer or is a process. Multiple answer optimisations were considered since it is the market reality. Some world class manufacturers utilise a group of factors that allows them to be successful, therefore looking for an "optimal solution" in this context is meaningless (use of the gradient resolution algorithm does not apply to this context).

Table 6. *Geometric average of the differences between target and calculated value.*

Z1	Z2	Z3
1103.4	4.0	0.0
6364.2	1923.4	0.0
8.5	194.3	0.0
3961.4	2.0	0.0
2573.9	40.1	0.0
4787.4	50.4	0.0
5356.5	52.1	0.0

Optimisation model

The goal function is represented in terms of the quality penalty predicted, from the distance between the value ($\hat{y}$) predicted to it is specified nominal value (T).

$$\text{Min Z} = (T - \hat{y})^2 \qquad (2)$$

As multiple variables were used due to the real manufacturing environment, a geometric average was applied to define the Z value. the desirability function was defined as follows:

$$\text{Min } Z_1 = \left[\prod_{i=1}^{n} \left(\hat{y}_i - T_i \right)^2 \right]^{\frac{1}{k}} \qquad (3)$$

where i and k are defined by the number of same time variables to be optimised or to get closer to the target.

Given the input matrix $X_{3\times 9}$ and X_1, X_2, X_3, X_4,

X_1 to X_4 are the raw material data,

$$X_{3\times 9} = \begin{bmatrix} X_5 & . & X_{13} \\ m_5 & . & m_{13} \\ M_5 & . & M_{13} \end{bmatrix}, \qquad (4)$$

X_i the process parameter, m_i the lower limit specified (LSL), and M_i the upper limit specified (USL). The data for Equation (4) are available upon request .

Thus, written in a different way:

m_i (LSL) < X_i < M_i (USL), I being from 5 to 13.

If T_i is the specified nominal value of Y_i, the difference between them can be expressed in the modulus as $D_i = |Y_i - T_i|$. Studies have shown that $D_i < 1$ can be achieved for the majority of cases.

In summary, two main streams were adopted for the constraints: the process variables where the experience, machine restrictions, raw material, and quality indicators will guide to define both the lower and upper specification limits, the other being where the customer or market specifies or declares what is desirable as an acceptable range of results.

Given the model coefficient matrix:

$$\alpha_{1\times 7}, \beta_{13\times 7} = \begin{bmatrix} \alpha_1 & \beta_1 & . & \beta_{13\,j} \\ . & . & . & . \\ \alpha_7 & \beta_7 & . & \beta_j \end{bmatrix} \quad (5)$$

In equation 5 (written as a matrix) we have α, which is a constant and β, which is the coefficient for each factor.

The variables predicted can be defined as:

$$Y_1 = \alpha_{11} + \beta_{11}X_1 + \beta_{21}X_2 + ... + \beta_{i1}X_i$$
$$... \quad (6)$$
$$Y_7 = \alpha_{17} + \beta_{17}X_1 +$$
$$+ \beta_{27}X_2 + ... + \beta_{i7}X_i$$

Equation 6 is just a representation of the predicted value equation for Y_1 until Y_7, i being from 1 to 13 and j from 1 to 7.

The data of Equations (5) and (6) are available upon request.

Case study

As a practical example of the application, the customer can specify the yarn characteristics, which is common in industries where robust quality systems are in place. For example, a customer could ask for a 183 Dtex with 34 filaments to be used in circular knitting, or a technical service person could order a product from a plant with additional information: tenacity over 42 cN/tex, elongation within 22 and 24 and shrinkage around 14.From now on these data can be used as a target for the quality desired (T_i), the main goal being to find the possible machine parameters and raw material that will satisfy the objective function of Min Z and its constraints. In most cases the raw material will be used as a block due to availability at the warehouse, Its quality limits are normally supplied and checked by the QA. Running the evolutionary solver from excel, numerous possible results can be encountered. The need to explore or simulate how to process will react to a change is always present, those requests come from internal customers (departments within the company) and external customers (who actually consume/ buy the product). To illustrate the power of PLS modelling, ***Table 6*** shows Z values of the following: $Z1$, being the existing model that uses the fundamentals of mechanics with no optimisation run through the GA, $Z2$, a model using PLS with no optimisation run through the GA and finally $Z3$, a model using PLS and optimised with GA. Therefore, the functionality and efficacy of the modeling and optimisation is demonstrated.

Conclusions

When there is a complex system where variables interact and correlate with each other, PLS can be a quick and simple tool applied to generate models of historical data. The traditional regression approach requires non colinearity and/or experimental work, which can be expensive in a complex process, difficult to undertake, and most of the time it does not allow practical usage. It also requires exploitation time for analysis and the creation of a solid theoretical base. The PLS showed that data can be accumulated when process control and traceability systems require, and when a considerable volume of data is available, multiple regression analysis with PLS can be performed to generate modeling, which can be updated with new production data or process adjustments, providing a continuous improvement process. The theoretical foundation will support the modelling, eliminating intermediate calculus, which could be controversial.

Optimisations showed to be feasible in a texturing environment, which gives the current market an opportunity to reduce or eliminate empirical trials, bringing actual value to the process without generating major costs.

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